WORKBOOK FOR GAUSSIAN MODELING ANALYSIS OF AIR CONCENTRATION MEASUREMENTS

Bruce Johnson, Terrell Barry, and Pamela Wofford

September 1999

STATE OF CALIFORNIA
Environmental Protection Agency
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ORDER is a lovely thing;
On disarray it lays its wing,
Teaching simplicity to sing.
It has a meek and lowly grace,
Quiet as a nun's face.
Lo—I will have thee in this place!
Tranquil well of deep delight,
All things that shine through thee appear
As stones through water, sweetly clear.

Anna Hempstead Branch
From The Monk in the Kitchen

1 INTRODUCTION. The gaussian modeling and related procedures have been used to interpret and analyze air monitoring studies, primarily around methyl bromide applications, but also MITC and 1,3-dichloropropene. The back-calculation procedure itself has been used in the methyl bromide permitting program to classify different kinds of methyl bromide applications with respect to potential for methyl bromide to volatilize into the atmosphere.

1.1 **Purpose of this document**

1.1.1 **Scope**. This document relates to procedures used to model field applications, as distinct from applications to buildings (structural applications).

1.1.2 **Record.** Environmental Hazards Assessment Program (EHAP) has analyzed various studies, issues have arisen during these analyses, which have sometimes caused us to change our procedures. In addition, the USEPA has improved and upgraded the original ISCST model from version 1 to version 3. This document provides a summary of our current procedures.

1.1.3 **Consistency.** Because different people work on these analyses at different times and because new people may be recruited to perform these analyses, this document establishes consistency in analysis.

1.2 **Helpful knowledge**. The optimum combination of knowledge and skills are quantitative and computer skills. The following lists the most important knowledge and skills in performing these modeling analyses.

1.2.1 **Concepts**

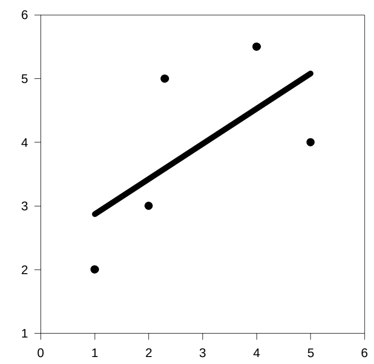
1.2.1.1 The relevant **mathematical and statistical** concepts can all be found in introductory textbooks.

1.2.1.1.1 regression

1.2.1.1.2 confidence intervals

1.2.1.1.3 trigonometry and geometry

1.2.1.1.3.1 sin, cosine, tangent, arctangent



Regression line through data points

1.2.1.1.3.2 angles-degrees versus radians

1.2.1.2 **Computer.** Different people accomplish the tasks associated with the concepts below in different way. Some use only the graphic user interface features of modern operating systems which include such programs as winfile, file manager, etc. Others continue to use the DOS concepts. In either case, it is helpful to understand the concept of path, subdirectory tree structures and ascii files, regardless of how you delete, rename and copy files.

1.2.1.2.1 DOS commands- copy, delete, rename, dos file names

1.2.1.2.2 ascii files

1.2.1.2.3 subdirectory tree structures

1.2.1.2.4 comma delimited data

1.2.1.3 **Physical science** - This area is mostly meteorology, though sometimes other physical sciences help us understand why a particular analysis isn't working very well. There are several references in EHAP which can help understand these concepts. They include Beychok (1994), Stull (1988), Turner (1994), Wark and Warner (1981) and Zannetti (1990).

1.2.1.3.1 boundary layer stability

1.2.1.3.1.1 inversion height

1.2.1.3.1.2 mixing height

1.2.1.3.1.3 temperature profiles

1.2.1.3.1.4 convective mixing

1.2.1.3.1.5 nighttime stable boundary layer

1.2.1.3.1.6 neutral stability

1.2.1.3.2 gaussian equation relating concentration to flux

1.2.1.3.3 log-wind speed profiles

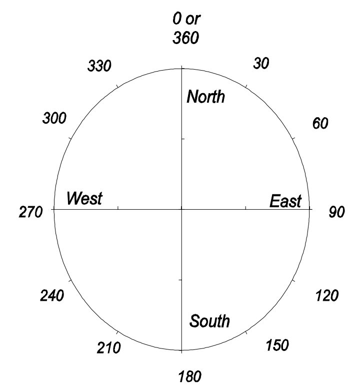
1.2.1.3.4 magnetic north, true north, angle of declination.

$$\tan(\theta) = \frac{\sin(\theta)}{\cos(\theta)}$$

$$57.3^o = 1.0 \ \textit{radian}$$

$$360^o = 2\pi \ \textit{radian}$$

An ascii file generally contains only printable characters such as numbers and letters.



1.2.2 **Specific software**. In conducting an analysis it is necessary to reformat tables of numbers, to import and export tables of numbers into various software, to perform regressions and make graphs. The following software helps to accomplish that. An alternative to some of this software is BREEZEAIR distributed by Trinity. It is supposed to automate some aspects of modeling and graphing.

1.2.2.1 EXCEL - spreadsheet, statistical analysis, some graphics (Microsoft Corporation)

1.2.2.2 Minitab - spreadsheet and statistical analysis (Minitab Inc)

1.2.2.3 DOS - operating system (Microsoft Corporation)

1.2.2.4 PE - ascii file editor (WordPerfect Corporation)

1.2.2.5 ISCST3 - the USEPA program for estimating air concentrations

1.2.2.6 WEATH5 - program by B Johnson for summarizing met data (Johnson 1999)

1.2.2.7 SUNFIX2 - program by B Johnson for obtaining sunrise/sunset times and sun angle (Johnson 1999)

1.2.2.8 RMAJAX - program by B Johnson for calculating regression and major axis regression (Johnson 1999)

1.2.2.9 Sigmaplot - plotting program (SPSS, Inc.)

1.2.2.10 Autosketch - cad/drawing program (Autodesk, Inc.)

Normally, wind direction is the 'from ' direction. A westerly wind is a wind from the west, from about 270 degrees. ISCST3 requires wind to be in the 'to' direction, 180 degrees offset from the 'from' direction.

1.3 Overview of procedure

1.3.1 **Estimate the flux density**. In most monitoring studies, you get air concentrations measured for some periods of time: 2 to 24 hours usually. Also provided are meteorological data such as wind speed and direction during the measurement periods. Using this information in conjunction with the physical layout of the samplers in relation to the field, you run the ISCST model to estimate air concentrations. Then you use the estimated air concentrations compared to the measured air concentrations to adjust the flux rate. The adjusted flux rate is the variable that is of major interest.

Flux and flux density. Physical chemists define flux as mass/area-time. Soil physicists use flux to mean mass/time (i.e. flow) and flux density to mean mass/area-time. In this workbook, flux and flux density will be used interchangeable and will mean mass/area-time.

We have arbitrarily decided to call this adjusted flux rate the 'flux index', in order to distinguish it from flux based on direct measurement.

What is flux? The units are mass per time per area. Typically such units would be ug/m^{2}s or lbs/acre-day. The concept expresses how much mass comes out of the ground and enters the atmosphere per unit area per unit time. Methyl bromide is shanked into the ground. A hollow tube conveys the methyl bromide from a tank on the tractor into the ground at some depth below the surface. The deeper the depth, generally, the lower the flux. Other factors affect flux, too, such as application rate. We have assumed, for example, that flux is proportional to application rate.

1.3.2 **Proportionality between flux and concentration**. The gaussian equation, which is the basis for the ISCST3 model, explicitly shows a proportional relationship between flux and concentration. That is, doubling the flux doubles the concentration. It is this proportional relationship between flux and concentration that enables the back calculation procedure. The procedure requires us to guess a flux rate to start with. The guess does not even have to be accurate, but we let the model estimate air concentrations based on that guess, then compare the modeled to measured concentrations to adjust our initial guess. That's how it works. Most of the time we use 100ug/m^{2}s (0.0001 g/m^{2}s) as a starting guess.

$$C = \frac{FK}{2\pi U_s} \int_x \frac{VD}{\sigma_y \sigma_z} \left(\int_y \exp\left[-0.5 \left(\frac{y}{\sigma_y} \right)^2 \right] dy \right) dx$$

$$C = FP$$

The first equation is the full, gaussian equation which relates concentration, C, to flux, F, and meteorology, distance and height. With all meteorology fixed and equal to P, as in the second equation, then the proportionality between C and F is clear.

1.4 **Some useful conversion factors.**

Conversion Factors

To convert from Column 1 to Column 2 multiply Col 1 by		To convert from Column 2 to Column 1, multiply Col 2 by	
Factor	Column 1	Column 2	Factor
0.447	mph	m/s	2.24
10000	hectares	square meters	0.0001
0.405	acres	hectares	2.47
4047	acres	meters	0.000247
0.305	feet	meters	3.28
0.112	lbs/acre	g/m^2	8.93
112000	lbs/acre	ug/m^2	8.93e-6
1.30e-6	lbs/acre-day	g/m^2s	7.71e5
1.30	lbs/acre-day	ug/m^2s	0.771
454	lbs	grams	0.00220
86400	day	seconds	1.157e-5
0.01745	degrees	radians	57.3
0.258	ug/m^3 m.b.	ppb m.b.	3.88*
0.001	ppb	ppm	1000.

*methyl bromide at 25°C

815ug/m^3 = 210 ppb for methyl bromide at 25° C

210 ppb = 0.210 ppm

Two more conversions, which don't fit neatly into the table, Fahrenheit to Celsius (centigrade): C=(F-32)*5/9 gives Celsius from Fahrenheit and F=(C*9/5)+32 gives Fahrenheit from Celsius. To get Kelvin from Celsius, C+273=K and in the other direction, C=K-273.

Finally, it is sometimes necessary to convert from parts per billion (ppb) to ug/m^3. This conversion is both temperature and compound specific. At 25 degrees for methyl bromide convert ppb to ug/m^3 by multiplying by 3.88. Conversely, to convert from ug/m^3 to ppb at 25^o degrees for methyl bromide, multiply by 0.258. Just remember that 815ug/m^3 is equivalent to 210 ppb.

1.5 **Example used in this workbook.** The example presented in this workbook was an actual set of calculations to analyze the 'Oceano' methyl bromide study. The associated memos are contained in the Appendix. This example had aspects which could not be described as a textbook example. Nevertheless, the study shows real problems that arise in conducting these kinds of analyses.

2 **ASSEMBLE DATA** - Various data required for the analysis must be put into a form which can be used by the ISCST3 model.

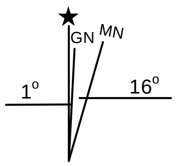
2.1 **Geographic data** (the geometry of the field and the sampler locations)

2.1.1 **Field location data**. Usually one starts with a map of the field. Determine if the units on the map are feet, meters or yards. Also determine where north is and whether north is defined as magnetic north or true north.

2.1.2 **Converting field location to coordinates**. Use the lower left corner of the field as coordinate 0,0. Arrange the two sides adjacent to this corner so that the vertical side is going up and down, and the horizontal side is going straight across. Many times, fields are rectangles, so this lining up is easy to do. However, sometimes fields are not rectangles. In the latter case, ideally the sides making up the lower left corner form a 90 degree angle. Then lining up this corner and these two sides will determine the rest of the field.

For the Oceano study, the lower left corner of the field is <u>not</u> a 90 degree angle (Figure 1). Consequently, the field has been represented as a series of 4 sub-rectangular areas (Figure 2). The coordinates used to generate Figure 2 and to perform the simulation are shown in Table 1.

2.1.3 **Field location in relation to direction.** The orientation of the field is important in order to be sure that the wind direction information is used correctly. Therefore, it must be clear whether north on the field map refers to magnetic north or true north. For example, along the central coast, the difference between magnetic north and true north is about 15 degrees. A measurement of 15 degrees with respect to true north would be equivalent to 0 degrees magnetic north along the central coast of California. While the ISCST3 has features which allow field rotation, it is important to understand the fundamentals behind the necessity for rotation and therefore, this workbook takes a more hands on approach. In this example, both the field directions and the wind directions were all measured in relation to magnetic north. Therefore, no rotation or adjustment of any angles was necessary.



Angle of declination (difference between truth north and magnetic north) can be found at the bottom of the USGS quad maps. GN is true north. MN is magnetic north. In this case, the declination is 16°.

A good way to check your coordinates for each corner of the polygon which makes up the field is by inputting those coordinates into Sigmaplot (or AutoSketch) and drawing the field. The resulting shape should approximate the map. Compare Figure 1 and Figure 2.

2.1.4 **Air sampler location data**. Each sampler location also receives a coordinate position. There must be enough information on the original map to ascertain these coordinates. As with the field coordinates, the sampler locations can be entered into Sigmaplot as a check against the original study map (Table 2). Compare Figure 1 and Figure 3. Each sampler will have a sampler height, the distance above ground. This is typically 1.2m (Table 2)

2.2 **Chemical monitoring data**. Generally chemicals are monitored for periods of time ranging from 2 to 24 hours. It is important to note that any concentration which results from such monitoring is an average concentration over that period of time. The wind direction shifts. The flux changes. Other conditions change. The instantaneous concentration probably resembles a messy wave function during the period of monitoring. However, the result of the chemical analysis is a single value for the entire time period, which represents the average concentration. Average concentrations for the example are shown in Table 3. Note that the concentration units are ppm (parts per million). When samplers quit operating during a monitoring period, a general guideline is to use the data if the sampler operated for at least 70% of the time period (Johnson 1999).

Samplers usually can not all be started at the same time. The field crew travels in a circuit to the sampling stations to change the sampling tubes. In order to define a sampling period when sample start times may range over a half an hour, utilize the average of the start and average of the end times. This may be rounded off to the nearest half hour.

2.3 **Meteorological data.** In most cases, onsite meteorological data will have been collected. This data will usually consist of temperature, wind speed and direction, sometimes humidity, precipitation, or standard deviation of wind direction.

2.3.1 **Wind speed**. The ISCST3 program requires wind speed in meters per second. The WEATH5 program converts wind speed in mph to meters per second. If you run wind speed in m/s through WEATH5, you will get the wrong values.

2.3.2 **Wind direction**. Wind direction most of the time is understood to be the 'from' direction. A northerly wind means that the wind is blowing from the north to the south. However, the ISCST3 program requires wind direction to be the 'to' direction. If a northerly wind is measured (approximately 0 degrees), then ISCST3 needs a measurement of approximately 180 degrees, indicating what direction the wind is blowing towards (i.e. in this case, towards the south). Again, the WEATH5 program will perform conversion from 'from' to 'to' directions. Also important here, is the framework used to measure the wind direction. Was the framework with respect to magnetic north or true north? The field directions and the wind measurement directions ultimately MUST BE RECONCILED, so that both are in the same frame of reference. If the field is drawn with respect to magnetic north, then the wind directions must be provided with respect to magnetic north. If the field is true north and the wind directions are magnetic north, then the wind directions must be shifted to align properly with the field. Table 4 presents excerpted meteorological data for the Oceano study.

2.3.3 **Temperature**. ISCST3 requires temperature in degrees Kelvin. The WEATH5 program converts Fahrenheit to Kelvin.

2.3.4 **Time**. The time period must be known for each period in order to divide the meteorological measurements up into the periods of time when the chemical measurements were taken. Also, the meteorological measurements will probably have to be summarized for each hour. EHAP will typically take 12 or more measurements every hour of wind speed, wind direction, temperature. These 12 measurements will have to be summarized for each hour during the period of chemical measurement. WEATH5 performs this summary. In Table 4, measurements for this example study were recorded once per minute. You must be alert to the possibility that different sources of time data may reflect daylight savings time or standard time. If there are different time frameworks, then decide on a common time framework and convert all time units into that framework.

2.3.5 **Stability class** -- see section on stability class estimation

2.4 **Application data**. Application data does not directly enter into the modeling. However, it is important to know attributes about the application such as depth, start of application, duration of application, type of application, application rate and so on. Often the first period of monitoring includes a period of application. This tends to make it difficult to obtain meaningful regressions because the tractor is moving over the field and the flux rates are changing drastically as the application proceeds. In addition, interpreting the analysis frequently depends on understanding the application factors. See Appendix for description of the application for the example study.

2.5 **Soil and vegetation data**. As with the application data, soil and vegetation data does not directly enter into the modeling process. Nevertheless, soil measurements such as bulk density, soil moisture, and organic matter content and vegetation type and percent cover, can sometimes help in interpreting the analysis of a pesticide application.

3 WEATHER SUMMARY PROCEDURES

3.1 **Format required by ISCST3.** The fixed format which ISCST3 uses is explained on pages 3-66 to 3-69 of the ISCST3 manual. Key points to remember are the units required by ISCST3 (meters/second, Kelvin) and that wind is expressed in degrees in the ‘to’ direction. Also remember that the framework for wind direction must be the same as the framework for the field and monitor coordinates, both must be with respect to true north or both with respect to magnetic north.

3.2 **How to get data into ISCST3 format**. The WEATH5 program handles much of the conversion and formatting required by ISCST3 from raw meteorological data collected by EHAP. WEATH5 is located on I:\airmodel and can be run by typing into a DOS window: *I:\airmodel\weath5.exe*. WEATH5 requires two input files, a raw met data file with comma delimited data in a certain order and in certain units (Table 5) and a cut file, which contains the date and hour for each time period for which a summary is required (Table 6).

The raw data file consists of mm,dd,hh,mi,int,at,agt,dir,spd where commas separate values and mm=month, dd=day, mi=minute, int=interval code, at=ambient temperature (F), agt=above ground temperature, dir=’from’ direction, spd= wind speed (miles per hour). ‘Int’ and ‘agt’ are not used, but there must be place holders in the file. The input file must be sorted from oldest to newest. WEATH5 produces output file giving time interval, average ambient air temperature in degrees Kelvin, average wind direction ‘to’ (mod(180+FROM,360)), scalar average wind speed (meters/second=.447*milesperhour). The data file can usually be prepared for WEATH5 input by using EXCEL and creating a ‘CSV’ (comma separated values = comma delimited) file, which is comma delimited.

City	*Latitude (deg-min)*	
Sacramento	*38º*	*34′*
San Francisco	*37º*	*46′*
Fresno	*36º*	*46′*
Monterey	*36º*	*36′*
Visalia	*36º*	*20′*
Orange	*33º*	*48′*

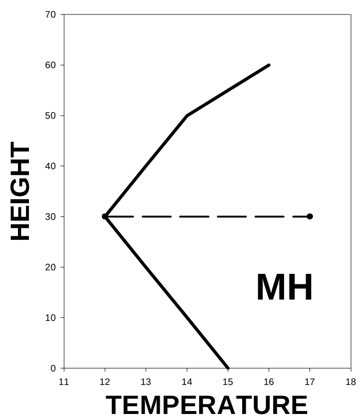
The cut file contains a listing of month, day, hour, minute, each separated by commas for each time period desired to summarize. The cut file can be created using EXCEL or Minitab (Table 6).

The output from the WEATH5 program for the meteorological data in the example is shown in Table 7. In order to run WEATH5, you must input the mixing height in meters. You must also know when sunrise and sunset occurs.

This can be determined from running the SUNFIX2 program (*I:\airmodel\sunfix2*) or you can also determine these times by running a program on the Naval Observatory Web site (*http://aa.usno.navy.mil/AA/*). In order to run these programs, you need to know the latitude of the site and the date. The Navy website has latitude information for most cities by name. Table 8 lists output from SUNFIX2 for 38.5º, the latitude of the Oceano study and output from the US Navy Astronomical Website.

The WEATH5 output provides the temperature values, wind direction and wind speed values which can be used for ISCST3 modeling. In addition, WEATH5 will produce an ISCST3 compatible met file, where only the stability has to be filled in (Table 9). The stability category field in WEATH5 ISCST3 compatible met file is indicated by the letter 'X'. These Xs need to be replaced by a number 1 through 6 to indicate the stability class.

3.3 **Stability.** Stability is a critical component of the meteorological input to ISCST3. Stability refers mostly to vertical mixing within the boundary layer. During a sunny day, the solar radiation heats up the ground, which heats up the air. This causes parcels of air to become less dense and rise like bubbles through the heavier, cooler air above. In turn, cooler air moves downward to displace the rising parcels. The degree of vertical mixing is captured in a six unit scale, sometimes using letter A through F, or using numbers 1 through 6. The code A connotes maximal vertical mixing, such as might take place on a sunny, summer day in the afternoon. The code F connotes night time stable conditions, when there is a temperature inversion at the surface and almost no vertical mixing. A temperature inversion at the surface means that coldest air is at the bottom next to the ground. Since the coldest air is also the most dense, there is no mixing. Stability condition D is neutral stability, where the temperature remains approximately the same over some vertical distance. This occurs during cloudy conditions, day or night. The remaining stability classes are in between these



Idealized temperature profile under convective daytime mixing conditions. MH indicates mixing height at dashed line.

classes. In the gaussian model, the stability class influences how quickly the downwind plume spreads out in a vertical and horizontal direction. Under F stability, the plume remains concentrated and tight for long distances. Under A stability, the plume readily spreads out, and consequently, concentrations decline more quickly down wind.

3.4 **Determining stability.** There are many procedures for determining stability. For this workbook, the procedure presented is the one we have used most often for site specific monitoring studies (Budney 1977). It requires knowledge of sunset and sunrise times, and the sun's angle above the horizon on an hourly basis. The sun angle above the horizon can be derived from either SUNFIX2 program or from the naval observatory web site [*http://aa.usno.navy.mil/AA/*]. In the latter case, choose under data services, 'Positions of sun and moon', then choose 'altitude and azimuth of the sun or moon during one day', then fill out the online form. In this case, if you know a reasonably large city nearby, the program will tell you the latitude and longitude, in addition to calculating the angles. For the SUNFIX2 program, you will also need the Julian day of the study.

Under Clear Sky Conditions

Category	***Sun Elevation Angle***
Strong insolation	*SEA > 60º*
Moderate insolation	*35º < SEA < 60º*
Slight insolation	*15º < SEA <35º*

Once you have obtained the sun angles, you should probably write them down next to each hour on the WEATH5 output. Then label the hours for night and day. The SUNFIX2 program goes by sun position to determine night/day. If the sun is above the horizon, it is day, otherwise it is night. EPA rules, however, require night to extend one hour after sunrise and start one hour before sunset. The WEATH5 program labels the hours night/day, using the user input sunset/sunrise times and also using the EPA rule of hour after and hour before. One thing to keep in mind, the times used either on the naval observatory web site or with the SUNFIX2 program, are standard time. Therefore, if the study times are all in daylight savings time, the hours must be adjusted. For example, if the SUNFIX2 program and the naval web site indicate a sunset time of 7:35 PM on June 30, that would correspond to a study time of 8:35 PM for a study where all

Stability categories

A	*1*	*very unstable*
B	*2*	*unstable*
C	*3*	*unstable*
D	*4*	*neutral*
E	*5*	*stable*
F	*6*	*very stable*

of the times were recorded as Pacific Daylight Savings time (which would probably be the case).

After writing down the sun angles, each hour during the daytime can be classified into strong, moderate or slight solar insolation. If there is any cloud information, these categories can be modified (see Table 10). A fully cloudy situation is D stability. Next start with the first hour. Assign the stability based on night/day, solar insolation (if daytime), and wind speed (Table 10). Another rule that should be followed: do not change the stability class from hour to hour by more than 1 stability class. For example, if stability class at hour 9 is E, then stability class at hour 10 can only be F, E or D. The stability classes are not allowed to jump or skip classes from hour to hour.

An alternative method for determining stability class requires the standard deviation of wind direction. Further references and a meta-code for this procedure can be found in Johnson (1998).

After inputting the stability classes, the weather file is ready for use by ISCST3.

4 RUN ISCST3

4.1 **Overview**. There are two files needed to run ISCST3: a control file and a meteorological data file. The control file contains the name of the meteorological data file, which is how the ISCST3 programs finds out about it. The control file contains various specifications on how to conduct the simulation. Some important elements are the source geometry (field coordinates), the receptor geometry (in this case, the coordinates of the monitor locations), the source information (sometimes the whole field, sometimes the whole field divided into subsources) which includes the flux rate, the name of the meteorological file, and the name of any output files, as well as other information and controlling parameters. Table 11 presents an annotated control file. The ISCST3 manual has extensive discussion of how to build such a control file. The easiest way to get going is to modify an existing control file which reflects a similar kind of simulation.

TIP: ASCII files can be edited using word perfect with courier font and ***be sure to "save as" an ascii file.***

4.2 **Run ISCST3.** To run ISCST3 type in

I:\airmodels\iscst3 infile outfile

where infile is the control file and outfile is the output file.

4.3 **Interpreting error messages**. When something is wrong with the control file, ISCST3 gives you an error message. ISCST3 will NOT give you an error message if your frame of references for wind direction and field locations are different. ISCST3 has no way of knowing that. However, if ISCST3 thinks that some of your specifications are inconsistent or missing, it will let you know. In general, you should spend 15-20 minutes trying to solve these error messages by iteratively reading the manual, modifying your control file and rerunning it. This procedure will help get you acquainted with the manual and help you discover other useful program features. After about 20 minutes, however, go ask for help from somebody who is more experienced.

TIP: Construct filenames that mean something. OCFIP1.IN, OCFIP1.OUT, OCFIP1.MET might indicate Oceano study, flux index, period 1 control file (input), output file and meteorological file.

4.4 **Checking output**. When you are starting a series of similar runs, for example, the first period of a 6 measurement period simulation, it is a good idea to print out your output file and look it over. Check the met data. Check the receptor and field coordinates and the source information. Look at the various control parameters. The program reprints and interprets the control information which is in your control file. You can determine if the program is correctly interpreting it by looking at the output.

For subsequent periods, probably the only part of the control file that will change will be the title and the met data file. Use the title to help document what you are doing: e.g. ‘Period 4, Oceano’ for example. It’s almost guaranteed that you or somebody else will have to come back someday and look at that control file. So it's a good idea to provide in the control file as much information as possible concerning the purpose of the simulation and related explanatory documents.

5 **COMPARING SIMULATED CONCENTRATIONS TO MEASURED CONCENTRATIONS**. This gets to the main purpose of performing these simulations. Trying to estimate or 'backcalculate' the flux rate. In this part of the procedure, the modeled and measured values are compared and through the comparison, the assumed flux rate is adjusted to more accurately reflect the 'real' flux rate. In order to distinguish a backcalculated flux from measured flux, we have decided to use the phrase "flux index" to connote estimates of flux derived from analysis of modeled air concentrations compared to measured values.

flux index

5.1 Make sure that the measured values and the simulated values are in the *same* units.

5.2 **Regression.**

5.2.1 **Major axis regression**. The natural method to use in order to calibrate the model flux rate to the measured concentrations is regression. For approximately 5 years, we have conducted regression using the measured values on the y-axis and the modeled values on the x-axis. For almost the same length of time, B.Johnson and T.Barry have discussed this issue, as to whether the modeled values should go on the x-axis or the y-axis. It can make a difference, particularly when the r-squared values are low. As a result of these discussions, we have decided to shift over to major axis regression (Johnson 1999). This is a kind of regression which expresses the functional relationship between two variables and is independent of which way the axis are arranged. When the r-squared value is high, it gives about the same result as regular regression. When the r-squared value is low, it gives a slope which is sort of the average between the two

In the Oceano study, four monitors ran for periods of time less than the full period (See Table 3). In two cases, the percent of time was less than 70%. The policy of excluding sampling results for monitoring samples less than 70% of the period was not in place. Reanalysis of interval 3 shows very little effect on the sorted normal regression (Johnson 1998).

INCLUDE SITE 6: Y=0.60X+0.
EXCLUDE SITE 6: Y=0.59X+0.

slopes one would derive by performing the regression first as x,y, then as y,x and taking the average of the x,y slope with the reciprocal of the y,x slope. It is still recommended, however, that the regression analysis be conducted with the measured values on the y axis and the modeled values on the x-axis. This workbook assumes that arrangement of axes.

5.2.2 **What do you do with regression.**

5.2.2.1 First step is to determine if the regression slope is significant. We have generally used a 5% significance level to decide this. There will be some relationship between the significance using normal regression and significance under major axis regression. The question, "Is the slope statistically significant" is equivalent to asking, "Does a 95% confidence interval around the slope include 0?" If the answer is no, then the slope is significant. If the answer to the latter question is yes, then the slope is not significant. The RMAJAX program gives slope confidence intervals for both normal regression and major axis regression slopes.

5.2.2.2 If the slope is significant, then you must also consider whether the intercept is significantly different from 0. Major axis regression does not provide a mechanism for determining whether the intercept is different from 0. Therefore, check the normal regression estimate of intercept. If the intercept is significant, but small in relation to the average measured values, then ignore it. If the intercept is statistically significant and large in relation to the measured values, consult with someone else to determine a course of action. Perhaps sensitivity analysis in the form of forcing the normal regression through the origin will indicate that the intercept does not affect the slope very much or perhaps there are peculiarities in the problem which logically cause the intercept term to appear. The ideal result at this point in the analysis is a statistically significant regression ($p<.05$) and a larger r^2 value (>90%) and a small and statistically non-significant intercept.

5.2.2.3 After obtaining the major axis slope, and assuming that the regression has been done with the measured values on the y axis and the modeled values on the x axis, then multiply the slope by 100, (or the flux rate that was used in the simulation). If you then resimulate using the new flux, you should get a regression slope close to 1.0. The implication is that you have estimated the flux for that period and produced what we are calling a 'flux index' for that period.

Table 12 shows the period 2 data and regression for the Oceano study. For this particular period, the normal regression slope was 0.5674 and the major axis regression slope was 0.60. Since the y values are the measured values and the x values are the modeled values, that means that the assumed flux index of 100ug/m^{2}s which was used to derive these modeled values, probably overestimates the actual average flux. Therefore, the assumed flux of 100ug/m^{2}s is multiplied by the coefficient of 0.57 to obtain a new flux index estimate of 57ug/m^{2}s.

The policy of using the major axis regression was not in place at this time the Oceano study was analyzed. Consequently, normal regression slope was used. Note also, the intercept in the normal regression was significant. However, further analysis of this difficult study indicated that the combined 24 hour TWA of 150 ug/m^{2}s (based on period 1 and 2 using 57ug/m^{2}s for period 2) was adequate for establishing the maximum required buffer zone (see Appendix).

5.2.2.4 If the slope is not significant, then you need to consider what to do when the regression doesn't work.

5.3 **What to do when regression doesn't work.** This is one of the hardest areas of the procedure to set fixed rules. The first question to ask, is why didn't the regression fit. There are some standard reasons, for example, the first period may have been monitored during application which results in very uneven flux during the monitoring period. But sometimes, the answer is simply, "I don't know." The rest of this section lists some techniques that have been thought about and/or used in this situation.

5.3.1 **Redo simulation using shorter time intervals for the meteorological data.** The idea here is that wind variation is not picked up in the hour long summaries and a better fit might be produced by finer resolution wind data. Despite its appeal, this approach has not proved very helpful in the past.

5.3.2 **Sort values and regress**. Sort the x values and the y values independently, then rerun the regression. In the Oceano example, the additive constant was highly significant and was large, compared to the measured values under regular regression. Therefore, I [B. Johnson] felt something more had to be done.

5.3.3 **Force sorted regression through the origin**. In the Oceano study, I [B. Johnson] redid the regression, using a Minitab option to force the regression through the origin.

5.3.4 Another procedure that may have been used previously was to simply **sum up the measured values**, divide by the sum of the modeled values and use that quotient to adjust the modeled flux rate.

5.3.5 **Substitute another period.** When meteorological conditions are similar and concentrations are similar, it may be reasonable to substitute the flux index from another period.

6 **COMPUTE AVERAGE FLUX INDEX FOR HIGHEST 24 HOUR PERIOD**. After determining the flux index for the individual periods, find a contiguous set of the highest flux periods, which add up to approximately 24 hours and determine the time weighted average flux index for those periods. This period will be the focus of further simulation. In the Oceano study, after revisiting the analysis to determine a flux index for period 1, the 24-hour time weighted average flux index was computed as follows:

$$weighted\ avg = \frac{11h \times 251\ \ \mu g/m^2 s + 12h \times 57\ \ \mu g/m^2 s}{23h} = 150\ \ \mu/m^2 s$$

__TIP__: Use the plot file feature of ISCST3 to create a data file containing the estimated concentrations, together with the x and y coordinates. Get into Sigmaplot, import the data from this file by specifying (1) white space separators (2) start in column 1 and go to column 3 (3) start in row 9 and go to the end. This will put the x,y,c (concentration) values into the first 3 columns of Sigmaplot. Then create a contour plot using those three columns.

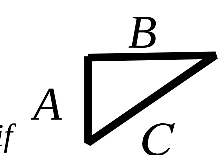
The flux indices from periods 1 and 2 were combined in a weighted average to estimate a 24 hour average flux index. In the Oceano study, this estimate was actually for a total period length of 23 hours. Sometimes the measured periods do not total to 24 hours.

7 **COARSE GRID SIMULATION.** To look for the maximum required buffer zone during the 24-hour period identified above, it is now necessary to simulate this 24 hour period, using the time weighted average flux index and the meteorological data associated with this time period. The first iteration of this procedure covers the field and surrounding area with a grid points in order to determine in which direction the highest concentrations go. Table 13 shows the control file for the coarse grid. Figure 4 shows

the contour plot using Sigmaplot to plot the points derived from the simulation output file called oc24h.p12 shown in Table 13.

8 **FINE GRID SIMULATION** This is the second, and sometimes third or fourth iteration of the procedure. The direction determined by the coarse grid is covered with a finer grid and the time period is resimulated in order to get a more exact estimate of the required buffer zone. The bufferzone is measured straight out from the sides when it's due west, east, north, or south of a rectangular field. However, it's measured from the corner when it's closest to a corner. Figure 5 shows the fine grid contour for the Oceano study, which focuses on the west side of the field where the highest concentrations occurred. Sometimes it is necessary to draw a line out to the maximum distance where 815 ug/m^3 is located and then measure the line. In this particular example, the location was very close to the horizontal axis and no line was necessary. But see tip for dealing with situations where the axis absolute units are different lengths. This distance is the required buffer zone for this 24-hour period.

TIP: Be careful in determining distance when the x and y axis have different absolute scales. For example, when 1 cm along the x axis represents 10m, while 1 cm along y axis represents 20m, you may have to use the Pythagorean theorem to determine the length of the hypotenuse.



In the diagram, if C is the length that we need to determine, then convert A and B into the axis units and use the following formula to find C:

$$C = \sqrt{A^2 + B^2}$$

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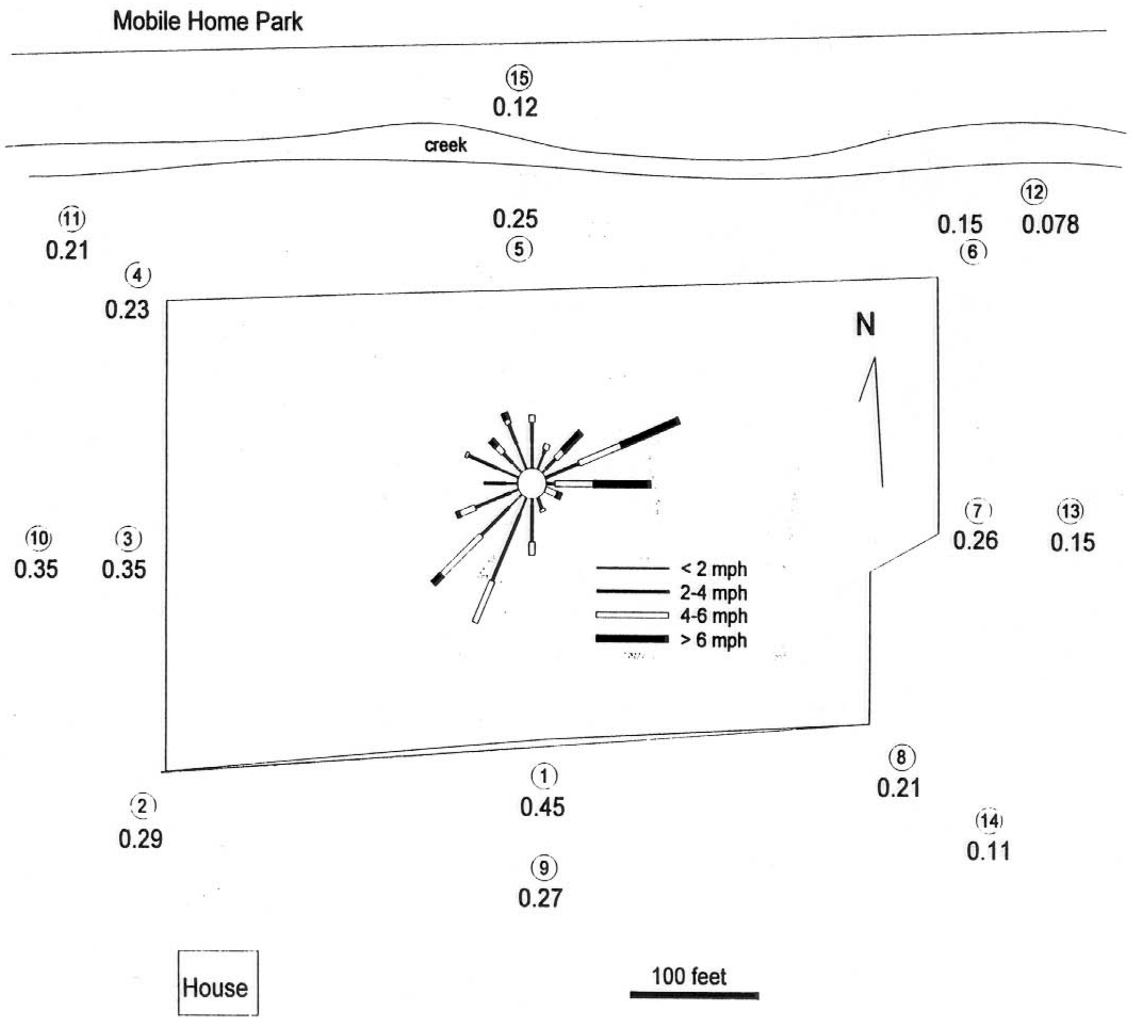
Figure 1. The application site, sampler positions, and the 23-hour time weighted average concentration (parts per million) and wind rose diagram for intervals 1& 2.



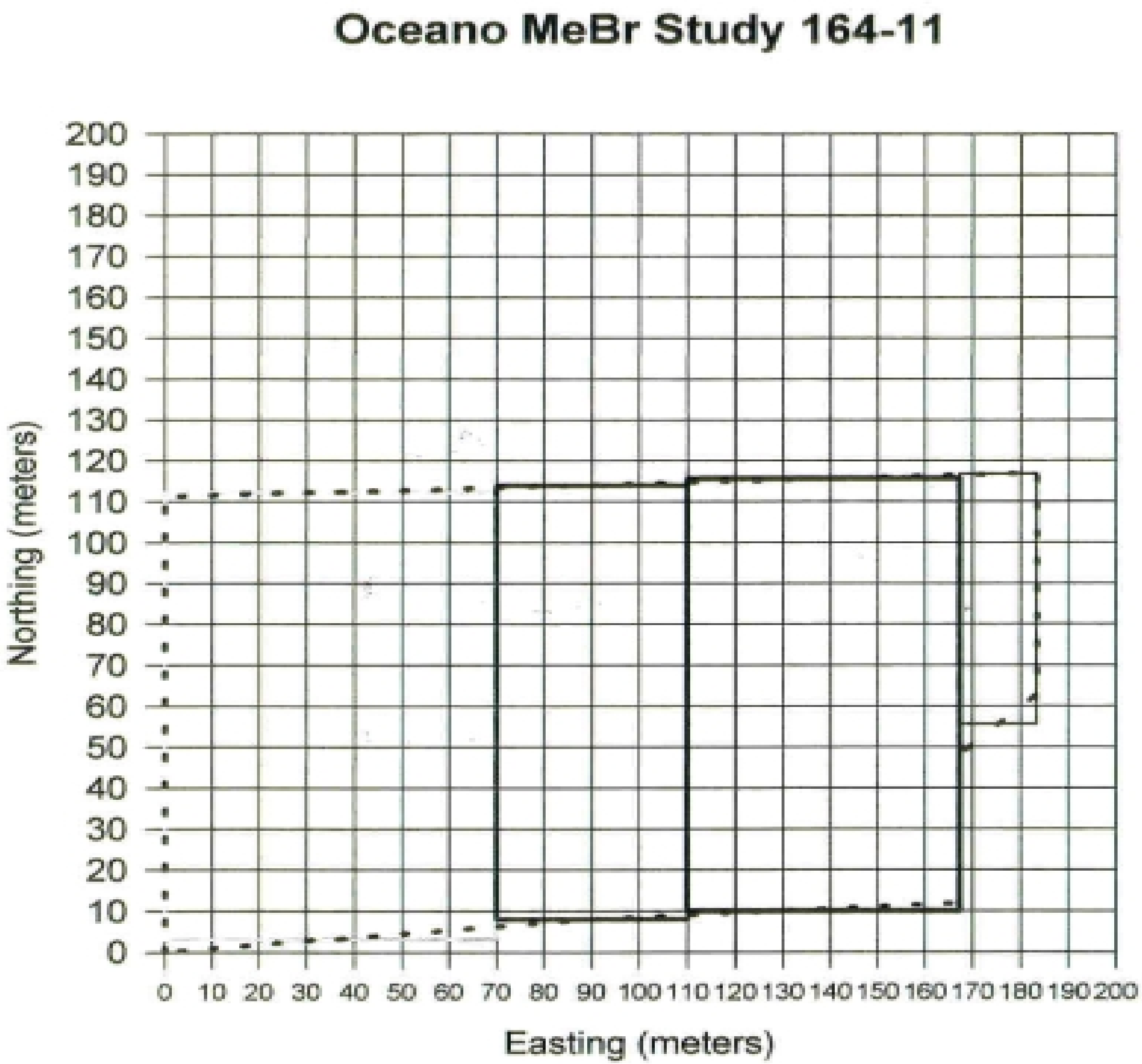


Figure 2. After determining coordinates of 4 sub-rectangles, this is sigmaplot drawn depiction of field. The dotted line represents the original field boundaries. ISCST3 requires rectangular sources.

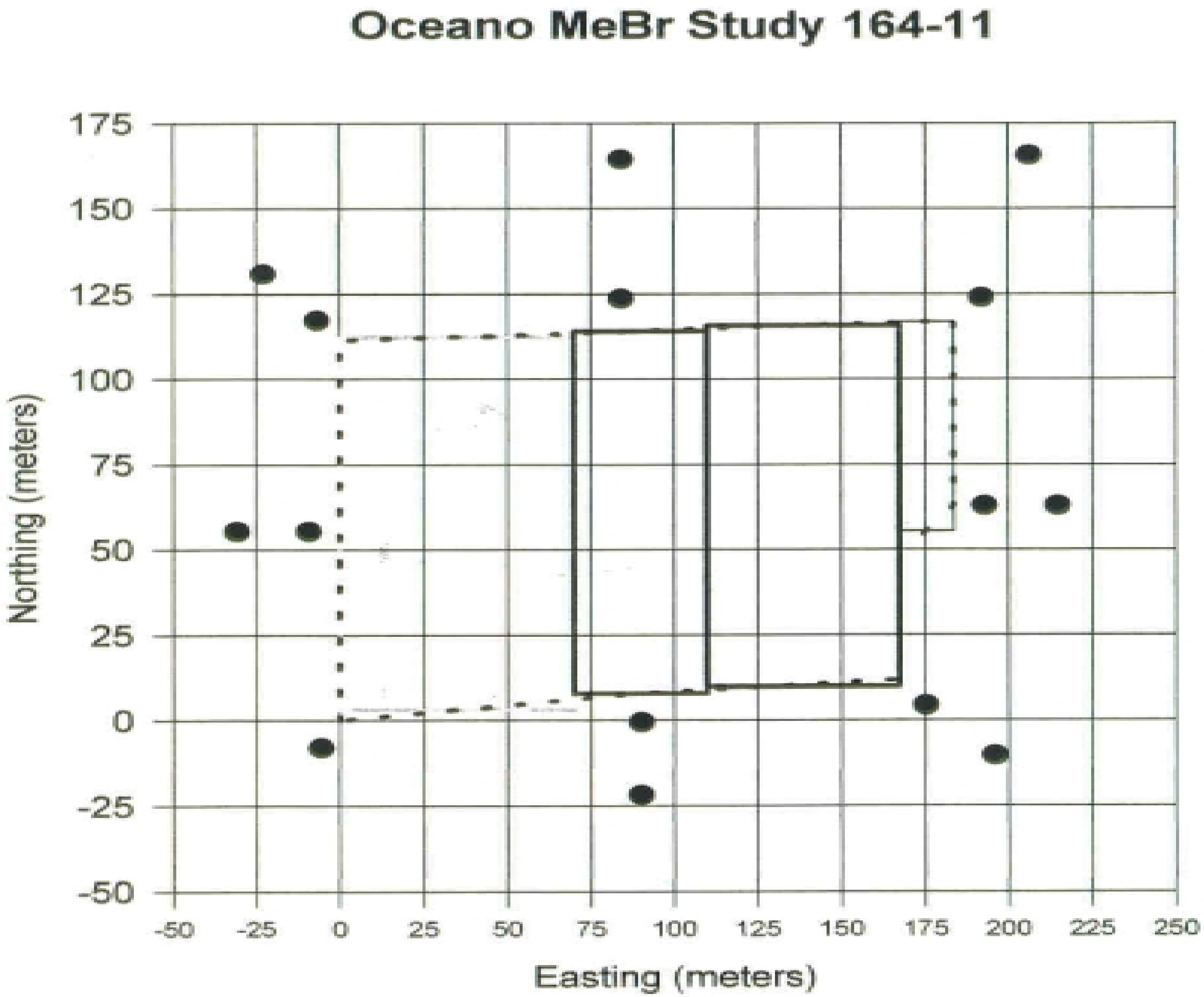


Figure 3. Sigmaplot drawn field map showing locations receptors.

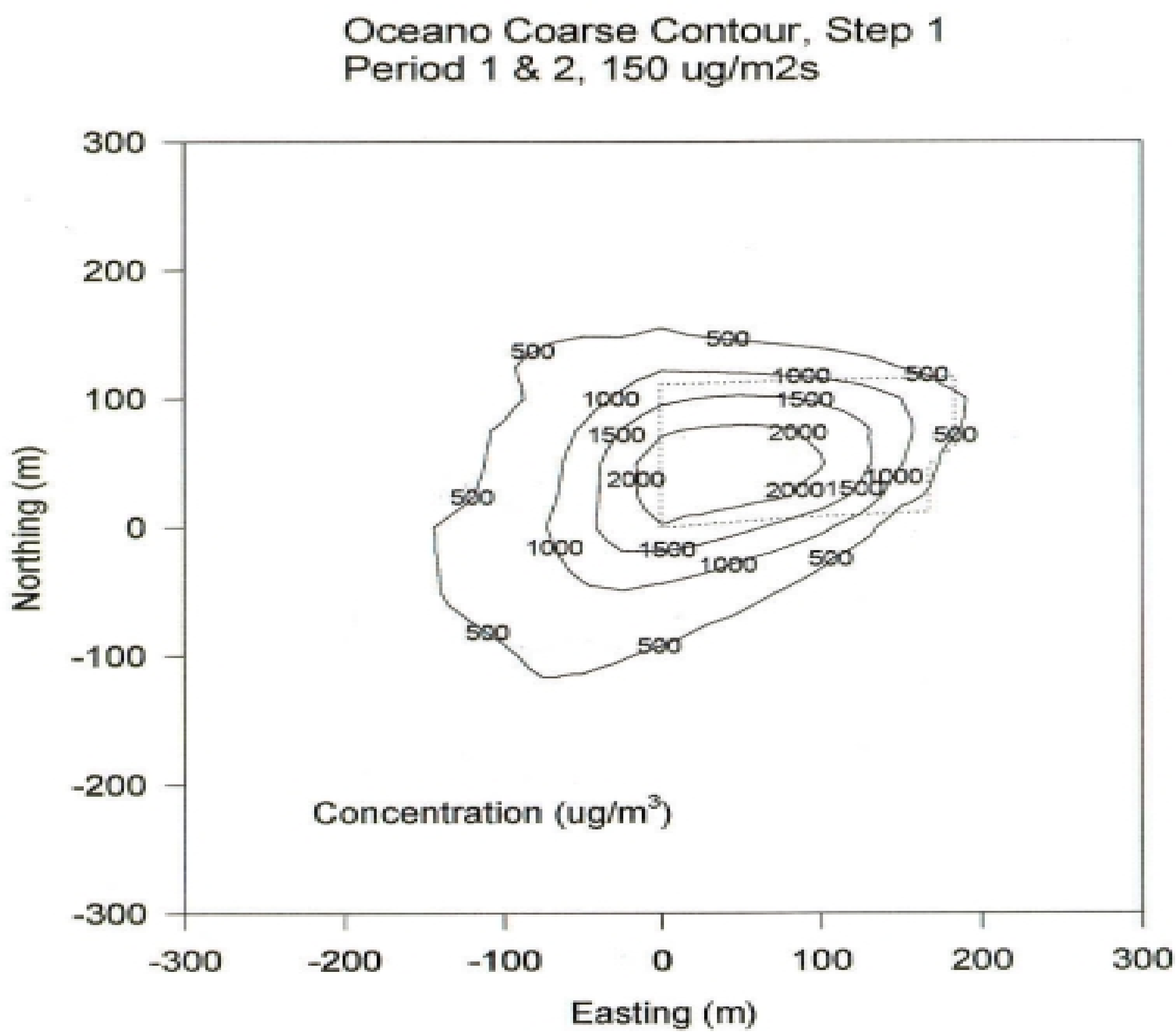


Figure 4. Coarse contour to locate direction of maximum buffer zone. Maximum direction west of field. Field indicated by dotted line in center.

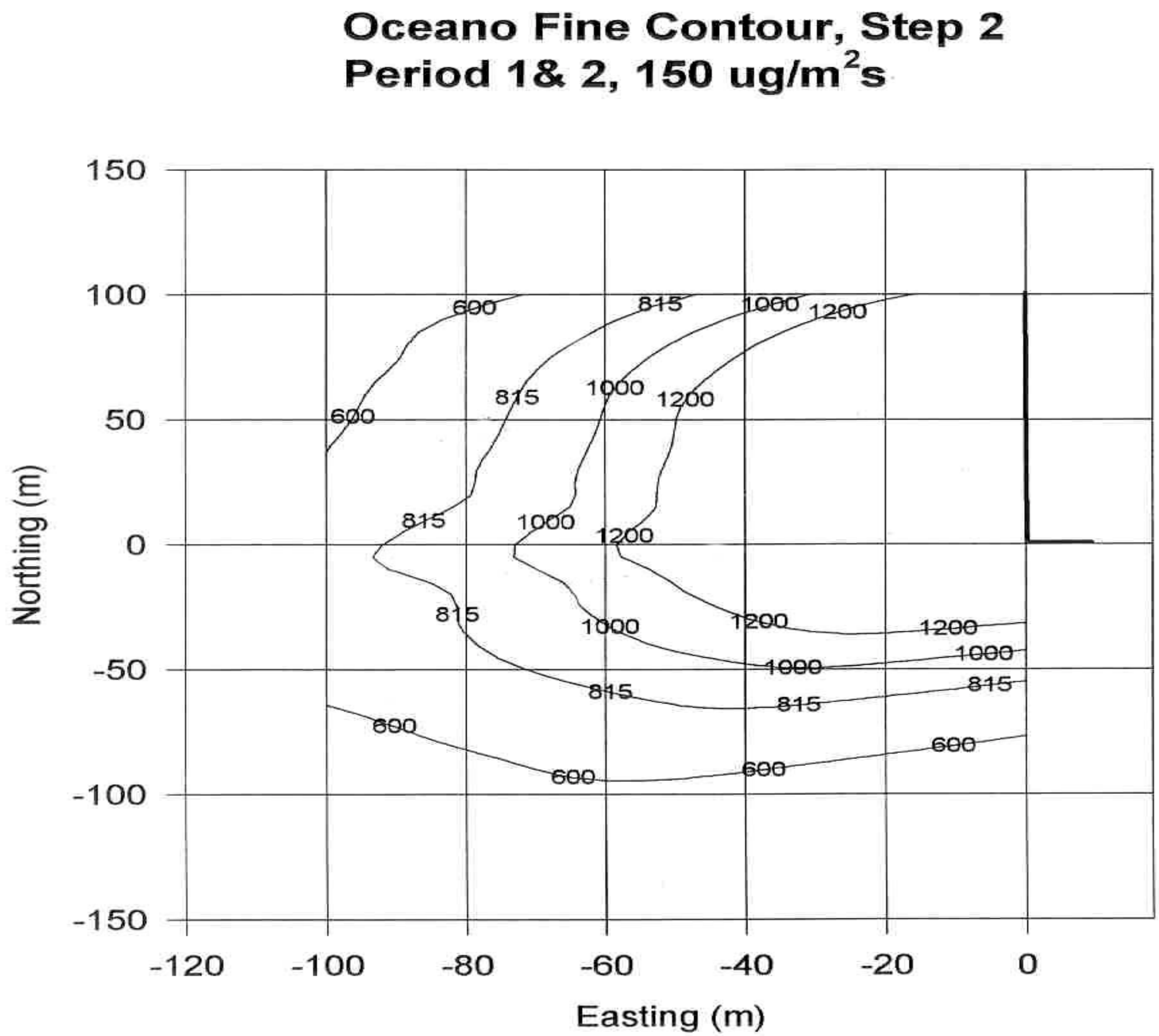


Figure 5. Finer grid to determine required buffer zone. Dark line indicates portion of west and southwest corner of field. Longest required bufferzone from SW corner to (-94,-5), giving length of 94m or 308 feet.

Table 1. Coordinates for boundaries of 4 rectangular subsources for field. All units are meters.

x-src 1	y-src 1	x-src 2	y-src 2	x-src 3	y-src 3	x-src 4	y-src 4
0.0000	3.1000	70.0000	7.9000	110.0000	9.9000	167.3000	55.5000
0.0000	112.3000	70.0000	114.0000	110.0000	115.6000	167.3000	116.8000
70.0000	112.3000	110.0000	114.0000	167.3000	115.6000	183.5000	116.8000
70.0000	3.1000	110.0000	7.9000	167.3000	9.9000	183.5000	55.5000
0.0000	3.1000	70.0000	7.9000	110.0000	9.9000	167.3000	55.5000

Table 2. Coordinates for receptors (monitors, locations where the monitors were set up).

x-recept	y-recept	height
90.2200	-0.6100	1.2000
-5.4900	-8.0800	1.2000
-9.1000	55.1700	1.2000
-6.7000	117.0000	1.2000
84.1000	123.4000	1.2000
192.0000	123.7000	1.2000
192.9400	62.8000	1.2000
175.3000	4.3000	1.2000
90.2000	-21.9000	1.2000
-30.8000	55.2000	1.2000
-22.9000	130.8000	1.2000
206.4000	165.5000	1.2000
214.9000	62.8000	1.2000
196.0000	-10.4000	1.2000
84.1000	164.3000	1.2000

Table 3. Ambient methyl bromide air concentrations (this is Table 1 from Kim and Segawa 1998).

		Methyl Bromide (ppm) for each sampling period					
		Interval 1	Interval 2	Interval 3	Interval 4	Intervals 1&2	Intervals 2&3
Site	Distance	11 Hour	12 Hour	12 Hour	12 Hour	23 Hour[1]	24 Hour[1]
1	28ft	**0.40**	**0.50**	0.072	0.12	**0.45**	**0.29**
2	32ft	0.17	0.39	0.011	0.11	0.29	0.20
3	30ft	0.20(89%)	0.48	0.041(72%)	**0.23**	0.35	0.26
4	30ft	0.14	0.30	0.056	0.14	0.23	0.18
5	33ft	0.27	0.23	**0.082**	0.088	0.25	0.16
6	34ft	0.25	0.062	0.029(63%)	0.014	0.15	0.046
7	31ft	0.32	0.20	0.058	ND(65%)	0.26	0.13
8	36ft	0.21	0.21	0.049	0.023	0.21	0.13
9	98ft	0.23	0.31	0.025	0.074	0.27	0.17
10	101ft	0.27	0.42	0.021	0.23	0.35	0.22
11	100ft	0.13	0.29	0.029	0.16	0.21	0.16
12	101ft	0.093	0.063	0.011	0.014	0.078	0.037
13	103ft	0.20	0.10	ND	0.016	0.15	0.052[2]
14	119ft	0.096	0.12	0.025	0.018	0.11	0.074
15	165ft	0.083	0.16	0.018	0.036	0.12	0.088

(%) Percentage of interval sampled is given for truncated sample periods, due to pump/battery failure during sampling interval.

[1] A two interval time weighted average concentration.

[2] indicates that the 24-hour average includes a period of no detectable amount, 0.0025ppm was used to obtain the 24-hour average.

ND = No detectable amount; reporting limit = 0.005 ppm

Bolded values are the highest concentrations for each column.

Table 4. Excerpt from EXCEL spreadsheet showing meteorological data. Battery is voltage. Int is period or interval. At is temperature (F). Dir is direction in degrees. Spd is speed in mph.

Batt	month	day	hour	min	int	at	agt	dir	spd
12.64	10	6	8	0	1	56.372	0	78.59	1.445
12.64	10	6	8	1	1	56.93	0	122.6	1.592
12.64	10	6	8	2	1	57.092	0	110.6	2.449
12.64	10	6	8	3	1	57.65	0	104.6	2.081
12.64	10	6	8	4	1	58.226	0	102.8	2.467
12.64	10	6	8	5	1	58.316	0	100.6	3.027
12.64	10	6	8	6	1	57.974	0	103.6	3.691
12.64	10	6	8	7	1	57.614	0	117.9	3.834
12.64	10	6	8	8	1	57.164	0	111.9	4.137
12.64	10	6	8	9	1	56.75	0	110.2	3.891
12.64	10	6	8	10	1	56.498	0	106.6	3.821
12.64	10	6	8	11	1	56.282	0	111.6	3.949

Table 5. Comma delimited file produced by exporting from Excel. This file contains the weather data from on site measurements, in preparation for analysis with WEATH5. The first line of headers is shown for illustration only. Before WEATH5 is actually run on this data, the first line below with the headers must be deleted so that the file only contains the data, separated by commas.

```
month,day,hour,min,int,at,agt,dir,spd
10,6,8,0,1,56.372,0,78.59,1.445
10,6,8,1,1,56.93,0,122.6,1.592
10,6,8,2,1,57.092,0,110.6,2.449
10,6,8,3,1,57.65,0,104.6,2.081
10,6,8,4,1,58.226,0,102.8,2.467
10,6,8,5,1,58.316,0,100.6,3.027
10,6.,8,6,1,57.974,0,103.6,3.691
10,6,8,7,1,57.614,0,117.9,3.834
10,6,8,8,1,57.164,0,111.9,4.137
10,6,8,9,1,56.75,0,110.2,3.891
10,6,8,10,1,56.498,0,106.6,3.821
10,6,8,11,1,56.282,0,111.6,3.949
```

Table 6. Excerpt from cut file, showing the hourly summaries desired from WEATH5. In the original met file, hours go from 0 to 23 and the cut file reflects this.

```
10, 6, 8,  0
10, 6, 9,  0
10, 6,10,  0
10, 6,11,  0
10, 6,12,  0
10, 6,13,  0
10, 6,14,  0
10, 6,15,  0
10, 6,16,  0
10, 6,17,  0
10, 6,18,  0
10, 6,19,  0
10, 6,20,  0
10, 6,21,  0
10, 6,22,  0
10, 6,23,  0
10, 7, 0,  0
10, 7, 1,  0
10, 7, 2,  0
10, 7, 3,  0
```

Table 7. Excerpt of WEATH5 output file for Oceano study.

```
WEATHER INPUT FILE: weathno.hed
oceana weather processing, add last 2 hours

USER DEFINED VALUES: SUNRISE@ 7:16, SUNSET@18:44
     NOTE THAT DAY STARTS 1 HR AFTER SUNRISE AND
     ENDS 1 HR BEFORE SUNSET FOR STABILITY CALCS
TODAY'S DATE: NOV 12 1998
        TIME: 13:52
      WEATH5: LAST MODIFIED 8/12/97. SCALER WIND SPEED,
      INCLUDES ALL WIND MSMNTS AND AVERAGE DIRECTION BASED
      ONLY ON MSMNTS WHERE SPEED> 0.5000MPH  [0.2235M/S].
------------------------------------------------------------
NAME OF ISCST3 MET DATA FILE: iscst3.tmp
------------------------------------------------------------
```

.......TIME PERIOD.........	SCA AVG TEMPERA K	180+AVG DIRECTI	SCA AVG SPD M/S	NUMBER OF RECORDS	N/D
10/ 6 8: 0 TO 10/ 6 9: 0	287.613	294.911	1.166	[60]	DAY
10/ 6 9: 0 TO 10/ 6 10: 0	292.571	351.861	1.216	[60]	DAY
10/ 6 10: 0 TO 10/ 6 11: 0	296.721	344.259	2.194	[60]	DAY
10/ 6 11: 0 TO 10/ 6 12: 0	298.633	72.752	2.708	[60]	DAY
10/ 6 12: 0 TO 10/ 6 13: 0	298.085	92.741	2.873	[60]	DAY
10/ 6 13: 0 TO 10/ 6 14: 0	298.057	89.419	3.388	[60]	DAY
10/ 6 14: 0 TO 10/ 6 15: 0	297.297	74.466	2.934	[60]	DAY
10/ 6 15: 0 TO 10/ 6 16: 0	296.915	80.533	2.737	[60]	DAY
10/ 6 16: 0 TO 10/ 6 17: 0	296.200	93.640	1.949	[60]	DAY
10/ 6 17: 0 TO 10/ 6 18: 0	297.268	79.319	1.722	[60]	DAY
10/ 6 18: 0 TO 10/ 6 19: 0	293.655	62.077	1.163	[60]	NIGHT
10/ 6 19: 0 TO 10/ 6 20: 0	289.859	261.281	0.821	[60]	NIGHT
10/ 6 20: 0 TO 10/ 6 21: 0	289.759	217.556	1.478	[60]	NIGHT
10/ 6 21: 0 TO 10/ 6 22: 0	287.673	213.778	0.959	[60]	NIGHT
10/ 6 22: 0 TO 10/ 6 23: 0	285.755	246.842	1.910	[60]	NIGHT
10/ 6 23: 0 TO 10/ 7 0: 0	286.858	229.546	1.552	[60]	NIGHT
10/ 7 0: 0 TO 10/ 7 1: 0	286.379	208.444	1.749	[60]	NIGHT
10/ 7 1: 0 TO 10/ 7 2: 0	283.943	282.476	0.964	[60]	NIGHT
10/ 7 2: 0 TO 10/ 7 3: 0	282.058	307.196	0.781	[60]	NIGHT
10/ 7 3: 0 TO 10/ 7 4: 0	283.278	246.925	1.065	[60]	NIGHT
10/ 7 4: 0 TO 10/ 7 5: 0	284.934	238.827	1.474	[60]	NIGHT
10/ 7 5: 0 TO 10/ 7 6: 0	282.948	262.624	1.460	[60]	NIGHT
10/ 7 6: 0 TO 10/ 7 7: 0	284.449	224.522	2.168	[60]	NIGHT
10/ 7 7: 0 TO 10/ 7 8: 0	284.236	237.221	2.008	[60]	NIGHT
10/ 7 8: 0 TO 10/ 7 9: 0	286.737	255.933	1.203	[60]	DAY
10/ 7 9: 0 TO 10/ 7 10: 0	289.401	325.267	1.229	[60]	DAY
10/ 7 10: 0 TO 10/ 7 11: 0	294.607	34.597	1.098	[60]	DAY
10/ 7 11: 0 TO 10/ 7 12: 0	293.586	100.017	3.702	[60]	DAY
10/ 7 12: 0 TO 10/ 7 13: 0	291.094	95.299	4.866	[60]	DAY
10/ 7 13: 0 TO 10/ 7 14: 0	292.715	88.299	3.691	[60]	DAY
10/ 7 14: 0 TO 10/ 7 15: 0	290.868	91.434	4.710	[60]	DAY
10/ 7 15: 0 TO 10/ 7 16: 0	291.237	103.151	4.616	[60]	DAY
10/ 7 16: 0 TO 10/ 7 17: 0	291.063	92.269	3.841	[60]	DAY
10/ 7 17: 0 TO 10/ 7 18: 0	290.555	55.686	2.857	[60]	DAY
10/ 7 18: 0 TO 10/ 7 19: 0	288.790	349.205	2.787	[60]	NIGHT
10/ 7 19: 0 TO 10/ 7 20: 0	287.626	295.521	2.301	[60]	NIGHT
10/ 7 20: 0 TO 10/ 7 21: 0	287.216	254.587	2.375	[60]	NIGHT
10/ 7 21: 0 TO 10/ 7 22: 0	286.694	223.199	1.714	[60]	NIGHT
10/ 7 22: 0 TO 10/ 7 23: 0	285.400	219.153	0.885	[60]	NIGHT
10/ 7 23: 0 TO 10/ 8 0: 0	284.059	257.508	0.664	[60]	NIGHT
10/ 8 0: 0 TO 10/ 8 1: 0	283.331	257.878	1.116	[60]	NIGHT
10/ 8 1: 0 TO 10/ 8 2: 0	283.057	247.805	1.262	[60]	NIGHT

Table 8. Output from sunfix2 for October 6, 1998 (Julian day 279).

LAT. DEG	DAY JUL	HOUR HR	SOLAR DEC DEG	SNSET ANGL DEG	SUNRIS HR DECHR	DAY LNGTH DECHR	SUN ELEV DEG	LIGHT DARK	SUN AZIM DEG
35.100	279	4	-6.071	85	6.3	11.43	-27	DARK	59
35.100	279	5	-6.071	85	6.3	11.43	-15	DARK	74
35.100	279	6	-6.071	85	6.3	11.43	-3	DARK	89
35.100	279	7	-6.071	85	6.3	11.43	8	LIGHT	104
35.100	279	8	-6.071	85	6.3	11.43	20	LIGHT	119
35.100	279	9	-6.071	85	6.3	11.43	30	LIGHT	134
35.100	279	10	-6.071	85	6.3	11.43	40	LIGHT	149
35.100	279	11	-6.071	85	6.3	11.43	46	LIGHT	164
35.100	279	12	-6.071	85	6.3	11.43	48	LIGHT	179
35.100	279	13	-6.071	85	6.3	11.43	46	LIGHT	194
35.100	279	14	-6.071	85	6.3	11.43	40	LIGHT	209
35.100	279	15	-6.071	85	6.3	11.43	30	LIGHT	224
35.100	279	16	-6.071	85	6.3	11.43	20	LIGHT	239
35.100	279	17	-6.071	85	6.3	11.43	8	LIGHT	254
35.100	279	18	-6.071	85	6.3	11.43	-3	DARK	269
35.100	279	19	-6.071	85	6.3	11.43	-15	DARK	284
35.100	279	20	-6.071	85	6.3	11.43	-27	DARK	299

Output from US Navy Astronomical Web Site

Oct.	Rise h m	Set h m
1	0557	1746
2	0558	1745
3	0559	1744
4	0600	1742
5	0600	1741
6	0601	1739
7	0602	1738
8	0603	1737
9	0603	1735
10	0604	1734

h m	Altitude o	Azimuth o
06:00	-1.1	95.6
07:00	11.1	104.4
08:00	22.6	114.4
09:00	33.2	126.3
10:00	42.0	141.6
11:00	47.9	161.0
12:00	49.6	183.6
13:00	46.4	205.6
14:00	39.4	223.6
15:00	29.9	237.7
16:00	19.0	248.8
17:00	7.3	258.3
18:00	-5.0	267.0

Table 9. ISCST3 compatible meteorological file outut from WEATH5. Field definitions are year,month,day,hour,to wind direction (degrees), scaler wind speed (m/s), temperature (K), stability class (all set equal to X), urban mixing height (m), rural mixing height (m). The mixing heights are arbitrarily set to 300m. The x's need to be relaced by estimate of stability class.

```
   99999        98   99999       98
9810 6 8 294.9111    1.1664 287.6 X   300.0   300.0
9810 6 9 351.8609    1.2163 292.6 X   300.0   300.0
9810 610 344.2586    2.1936 296.7 X   300.0   300.0
9810 611  72.7523    2.7084 298.6 X   300.0   300.0
9810 612  92.7406    2.8728 298.1 X   300.0   300.0
9810 613  89.4185    3.3880 298.1 X   300.0   300.0
9810 614  74.4658    2.9344 297.3 X   300.0   300.0
9810 615  80.5330    2.7372 296.9 X   300.0   300.0
9810 616  93.6403    1.9486 296.2 X   300.0   300.0
9810 617  79.3186    1.7215 297.3 X   300.0   300.0
9810 618  62.0765    1.1630 293.7 X   300.0   300.0
9810 619 261.2809    0.8206 289.9 X   300.0   300.0
9810 620 217.5560    1.4783 289.8 X   300.0   300.0
9810 621 213.7779    0.9587 287.7 X   300.0   300.0
9810 622 246.8420    1.9100 285.8 X   300.0   300.0
9810 623 229.5460    1.5516 286.9 X   300.0   300.0
9810 624 208.4444    1.7488 286.4 X   300.0   300.0
9810 7 1 282.4759    0.9637 283.9 X   300.0   300.0
9810 7 2 307.1960    0.7806 282.1 X   300.0   300.0
9810 7 3 246.9253    1.0652 283.3 X   300.0   300.0
9810 7 4 238.8274    1.4737 284.9 X   300.0   300.0
9810 7 5 262.6243    1.4596 282.9 X   300.0   300.0
9810 7 6 224.5218    2.1684 284.4 X   300.0   300.0
9810 7 7 237.2213    2.0080 284.2 X   300.0   300.0
9810 7 8 255.9327    1.2027 286.7 X   300.0   300.0
9810 7 9 325.2673    1.2288 289.4 X   300.0   300.0
9810 710  34.5973    1.0976 294.6 X   300.0   300.0
9810 711 100.0170    3.7022 293.6 X   300.0   300.0
9810 712  95.2991    4.8662 291.1 X   300.0   300.0
9810 713  88.2989    3.6910 292.7 X   300.0   300.0
9810 714  91.4341    4.7099 290.9 X   300.0   300.0
9810 715 103.1510    4.6164 291.2 X   300.0   300.0
9810 716  92.2686    3.8409 291.1 X   300.0   300.0
9810 717  55.6863    2.8567 290.6 X   300.0   300.0
9810 718 349.2053    2.7874 288.8 X   300.0   300.0
9810 719 295.5209    2.3013 287.6 X   300.0   300.0
9810 720 254.5872    2.3749 287.2 X   300.0   300.0
9810 721 223.1991    1.7141 286.7 X   300.0   300.0
9810 722 219.1534    0.8847 285.4 X   300.0   300.0
9810 723 257.5083    0.6641 284.1 X   300.0   300.0
9810 724 257.8778    1.1156 283.3 X   300.0   300.0
9810 8 1 247.8049    1.2621 283.1 X   300.0   300.0
9810 8 2 258.6865    1.7618 281.8 X   300.0   300.0
9810 8 3 233.9922    0.9797 281.6 X   300.0   300.0
9810 8 4 224.3038    0.9579 281.2 X   300.0   300.0
9810 8 5 249.0121    1.0130 281.2 X   300.0   300.0
9810 8 6 270.6490    0.9701 280.3 X   300.0   300.0
9810 8 7 252.9096    1.0087 282.2 X   300.0   300.0
```

Table 10. Tables from Budney (1977) showing the Pasquill stability class determination based on wind speed, night/day, and solar insolation. The second table indicates how to convert information on cloud cover into solar insolation categories.

Surface Wind Speed at a Height of 10m (m/sec)	Day Incoming Solar Radiation* (Insolation)			Night	
	Strong	Moderate	Slight	Thinly Overcast or ≥ 4/8 Low Cloud Cover	≤ 3/8 Cloud Cover
< 2	A	A-B	B	F	F
2-3	A-B	B	C	E	F
3-5	B	B-C	C	D	E
5-6	C	C-D	D	D	D
> 6	C	D	D	D	D

The neutral class (D) should be assumed for all overcast conditions during day or night.

*Appropriate insolation categories may be determined through the use of sky cover and solar elevation information as follows:

Sky Cover	Solar Elevation Angle > 60°	Solar Elevation Angle ≤ 60° But >35°	Solar Elevation Angle ≤ 35° But > 15°
4/8 or Less or Any Amount of High Thin Clouds	Strong	Moderate	Slight
5/8 to 7/8 Middle Clouds (7000 feet to 16,000 foot base)	Moderate	Slight	Slight
5/8 to 7/8 Low Clouds (less than 7000 foot base)	Slight	Slight	Slight

Table II. Annotated control file.

CONTROL

```
CO STARTING
CO TITLEONE Oceano period 1
CO MODELOPT CONC RURAL        NOSTD   NOBID NOCALM
CO AVERTIME PERIOD
CO POLLUTID OTHER
CO DCAYCOEF  .0000
CO FLAGPOLE 1.2
CO RUNORNOT RUN
CO ERRORFIL OCERR.OUT
CO FINISHED
```

RURAL SETTING

NO CALMS PROCESSING

SETS DEFAULT RECEPTOR HEIGHT

SOURCES

```
SO STARTING
SO LOCATION     1 AREA           0.000      1.100    0.000
SO SRCPARAM     1 .0001       0.0  70.   109.2  0.   0.
SO LOCATION     2 AREA           70.        7.9      0.
SO SRCPARAM     2 .0001       0.0  40.  106.1  0.    0.
SO LOCATION     3 AREA           110.       9.9      0.
SO SRCPARAM     3 .0001       0.0  57.3  105.7  0.  0.
SO LOCATION     4 AREA           167.3      55.5     0.
SO SRCPARAM     4 .0001       0.0  16.2  61.3  0.  0.
SO EMISUNIT   .10000E+7  (GRAMS/SEC)     (MICROGRAMS/CUBIC-METER)
SO SRCGROUP ALL
SO FINISHED
```

flux g/m²-s

x y lower left corner

y length

x length

METERS

FIRST OF FOUR SOURCE RECTANGLES

SOURCE DESCRIPTION

FACTOR TO CONVERT FROM G/S TO µg/m3

RECEPTORS

```
RE STARTING
RE DISCCART   90.22 -0.61 1.2
RE DISCCART  -5.49  -6.08  1.2
RE DISCCART -9.1  55.17 1.2
RE DISCCART -6.7 117.0 1.2
RE DISCCART 84.1 123.4 1.2
RE DISCCART 192.0 123.7 1.2
RE DISCCART 192.94  62.8 1.2
RE DISCCART 175.3  4.3 1.2
RE DISCCART 90.2  -21.9 1.2
RE DISCCART -30.8 55.2 1.2
RE DISCCART -22.9 130.8 1.2
RE DISCCART 206.4 165.5 1.2
RE DISCCART 214.9 62.8 1.2
RE DISCCART 196. -10.4 1.2
RE DISCCART 84.1 164.3 1.2
RE FINISHED
```

Y-COORDINATE

HEIGHT

RECEPTOR (MONITOR) LOCATIONS IN METERS

X-COORDINATE

MET DATA

```
ME STARTING
ME INPUTFIL OCEANo.P1        (4I2,2F9.4,F6.1,I2,2F7.1)
ME ANEMHGHT  10.000 METERS
ME SURFDATA  99999 1998        SURFNAME
ME UAIRDATA  99999 1998        UAIRNAME
ME WINDCATS   1.54 3.09 5.14 8.23 10.8
ME FINISHED
```

CONTAINS MET DATA FOR ISCST3

OUTPUT

```
OU STARTING
OU FINISHED
```

Table 12. Regression output from RMAJAX and comma separated data file listing used as input to RMAJAX for period 2 of Oceano study.

```
period 2, ppm
~~~~~~~~~~ORDINARY REGRESSION STATS~~~~~~~~~~
N=  15,SLOPE=    0.5674, INTERCPT=    0.1467
SYX=          0.06472, R2=  0.8144 ( 81.44%)
REGRESSION SSQ=           0.2390, RESIDUAL SSQ=          0.0545

F VALUE (1, 13) FOR REGRESSION =       57.05
 AND SIGNIFICANCE=   0.0000 (p<  0.00%)
XBAR=  0.192E+00 YBAR=  0.256E+00 STAN DEV X =  0.230E+00

SLOPE=  0.567E+00
SLOPE CI'S:    ** 99% ( 0.341E+00, 0.794E+00) -- 95% ( 0.405E+00, 0.730E+00)**

INTCPT= 0.1467E+00
INTCPT CI'S: **99% ( 0.803E-01, 0.213E+00) -- 95% ( 0.990E-01, 0.194E+00)**

FOR X=  0.000E+00, Y OF X=  0.147E+00
CI'S Y EST: ** 99% ( 0.803E-01, 0.213E+00) -- 95% ( 0.990E-01, 0.194E+00)**

~~~~~~~END OF ORDINARY REGRESSION STATS~~~~~~~~~~

^^^^^^^BEGINNING OF MAJOR AXIS REGRESSION STATS^^^^^^
N=   15, MAJOR SLOPE=    0.60028, INTERCPT=    0.14041
SLOPE CI'S:    ** 99% ( 0.381E+00, 0.873E+00) -- 95% ( 0.439E+00, 0.788E+00)**
MINOR AXIS SLOPE=   -1.66589
FIRST EIGENVALUE=          0.07107, SECOND E.V.=          0.00290
^^^^^^^^^^END OF MAJOR AXIS REGRESSION STATS^^^^^

------end of RMAJAX output---------------------------
```

Data file: P2.CSV showing measured,modeled concentrations (modeled concentration units were originally ug/m3, but converted to ppm by multiplying by 1/(1000*3.88)).

```
0.500,0.388307
0.390,0.582074
0.480,0.642368
0.300,0.211546
0.230,0.119558
0.062,0.000000
0.200,0.000000
0.210,0.000000
0.310,0.242724
0.420,0.496012
0.290,0.168515
0.063,0.000000
0.100,0.000000
0.120,0.000000
0.160,0.028086
```

Table 13. Annotated control file for coarse grid simulation. Flux rate set to 150 ug/m2s based on weighted average from periods 1 and 2. Meteorology file is combination of periods 1 and 2, resulting in 23 hours. In this simulation, control file requests special plot output to file 'OC24H1x.plt'. Use of this output option makes it easy to produce contour plots with sigmaplot, and probably other plotting programs.

```
CO STARTING
CO TITLEONE Oceano periods 1&2 23 hour simulation max buff
CO MODELOPT CONC   RURAL         NOSTD  NOBID NOCALM
CO AVERTIME PERIOD
CO POLLUTID OTHER
CO DCAYCOEF  .0000
CO FLAGPOLE 1.2
CO RUNORNOT RUN
CO ERRORFIL OCERR.OUT
CO FINISHED
SO STARTING
SO LOCATION    1 AREA              0.000     3.100    0.000
SO SRCPARAM    1 .000150     0.0  70.   109.2    0.   0.
SO LOCATION    2 AREA             70.          7.9      0.
SO SRCPARAM    2 .000150     0.0  40. 106.1  0.     0.
SO LOCATION    3 AREA             110.         9.9      0.
SO SRCPARAM    3 .000150     0.0  57.3  105.7  0.   0.
SO LOCATION    4 AREA             167.3       55.5      0.
SO SRCPARAM    4 .000150    -0.0  16.2  61.3  0.  0.
SO EMISUNIT   .10000E+7  (GRAMS/SEC)     (MICROGRAMS/CUBIC-METER)
SO SRCGROUP ALL
SO FINISHED
```

START X VALUE — DISTANCE BETWEEN POINTS

RECEPTOR GRID

```
RE STARTING
RE GRIDCART MAXBUF STA
              XYINC        -200 19 25   -200 19 25
RE GRIDCART MAXBUF END
RE FINISHED
```

OF PTS — Y RECEPTOR DESCRIPTION

```
ME STARTING
ME INPUTFIL OC24H.P12       (4I2,2F9.4,F6.1,I2,2F7.1)
ME ANEMHGHT  10.000 METERS
ME SURFDATA  99999 1998        SURFNAME
ME UAIRDATA  99999 1998        UAIRNAME
ME WINDCATS   1.54 3.09 5.14 8.23 10.8
ME FINISHED
```

MET FILE - COMBINED MET FOR PERIODS 1 & 2

```
OU STARTING
OU PLOTFILE PERIOD ALL OC24H1x.plt
OU FINISHED
```

PLOT FILE CONTAINING X,Y,C VALUES FOR INPUT TO PLOTTING PROGRAM

Appendix

dpr

Peter M. Rooney
Secretary for
Environmental Protection

Department of Pesticide Regulation

James W. Wells, Director
830 K Street • Sacramento, California 958 14-35 10 • www.cdpr.ca.gov

Pete Wilson
Governor

MEMORANDUM

TO: Douglas Y. Okumura, Acting Assistant Director
Division of Enforcement, Environmental
Monitoring and Data Management

FROM: David Kim, Environmental Research Scientist
Environmental Monitoring and Pest Management Branch
(9 16) 324-4340
Randy Segawa, Environmental Research Scientist
Environmental Monitoring and Pest Management Branch
(916) 324-4137

DATE: November 3,1998

SUBJECT: MONITORING RESULTS FROM A BEDDED TARPED, HIGH BARRIER FILM, SHALLOW INJECTION METHYL BROMIDE APPLICATION IN SAN LUIS OBISPO COUNTY

Introduction-Methyl bromide is widely used as a preplant soil fumigant for control of nematodes, fungi, diseases, and weeds. The Department of Pesticide Regulation (DPR) and county agricultural commissioners have implemented permit conditions, including buffer zones, to mitigate unacceptable methyl bromide exposure (greater than 0.21 parts per million; 24-hour time-weighted average). The buffer zone distances for this method have been determined from data received and evaluated by DPR to date. Additional monitoring was made to test and evaluate the effectiveness of the buffer zone distances.

Materials and Methods-The field monitored was treated with methyl bromide by a shallow bedded tarped application method on October 6, 1998. In this method the beds are formed prior to application. A methyl bromide/chloropicrin mixture is injected into the bed at a depth of six inches and immediately covered with a high density polyethylene (high barrier) tarpaulin and reshaped with the application rig.

The 7-foot wide tarpaulin covered the top and sides of the bed, the edges were buried at the base of the beds with the application rig. The beds were 4 feet wide with a 5 1/2-foot spacing. The field was located in Oceano, San Luis Obispo county.

The application site consisted of a 4.75-acre portion of a 9-acre field. A two acre portion of a field on the south border was treated with methyl bromide two days prior to the application. The buffer zone for this application was 100 feet based on a method 9.1 application. The application rate was 275 pounds per acre of formulated product, 75 percent methyl bromide 25 percent chloropicrin. Application took approximately 7 1/2 hours.

Ambient air samples were collected at 15 locations using activated charcoal tubes (SKC #226-38-02) and air samplers (SKC #226-38-02) calibrated at 15 milliliters per minute. Eight samplers were located approximately 30 feet, six at 100 and one at 165 feet from the treatment edge. Table 1 and Figure 1 indicate the position of each sampler. Samples were collected for four sampling periods beginning at 8:45 a.m., with the start of fumigation at 8:55 a.m. Samples were collected for one 1l-hour followed by three 12-hour periods, for a total of 47 hours.

The California Department of Food and Agriculture's Center for Analytical Chemistry conducted the laboratory analyses. These samples were extracted with ethyl acetate and analyzed using a gas chromatograph with an electron capture detector.

The weather was mostly sunny and clear skies with some high clouds in the afternoon. Temperatures ranged from 45 to 80 degrees Fahrenheit. The wind was generally from the west-southwest at 5 to 10 miles per hour from the late mornings to early evening, and from the northeast at 1 to 5 miles-per-hour at night (Figure 1).

Results-Off-site methyl bromide air concentrations exceeded DPR's target level of 0.21 parts per million (24-hour time weighted average) at the 100 foot resident buffer zone. The highest 24-hour time weighted average concentration at 100 feet was 0.35 parts per million at sampler 10. Samplers 9 and 11 also exceeded the target level at 0.27 and 0.21 parts per million. The highest 24-hour time weighted average concentration at 30 feet was 0.45 parts per million at sampler 1. The highest concentrations during a monitoring period were measured during interval 2, from 7:45 p.m. to 7:45 a.m. (Table 1 & Figure 1).

Air concentrations at the mobile home park located 195 feet from the north edge of the field were below the target level. Sampler 15- 30 feet from the mobile home park and 165 feet from the field, measured 0.12 parts per million. Samplers 11 and 12, 120 feet from the mobile home park and 100 feet from the field, had concentrations of 0.21 and 0.078 parts per million respectively. The air concentrations at the house 150 feet to the south of the field may have exceeded the target level. A sampler was not placed at the house, modeling of the data is required to estimate the air concentrations at the house.

Although methyl bromide air concentrations exceeded the target level, revised permit conditions, dated October 9, 1998, extend the residential buffer zone for this application from 100 to 450 feet (Enforcement Letter ENF 98-041).

Please contact either of us if you have any questions.

Figure 1. The application site, sampler positions, and the 23-hour time weighted average concentration (parts per million) and wind rose diagram for intervals 1& 2.

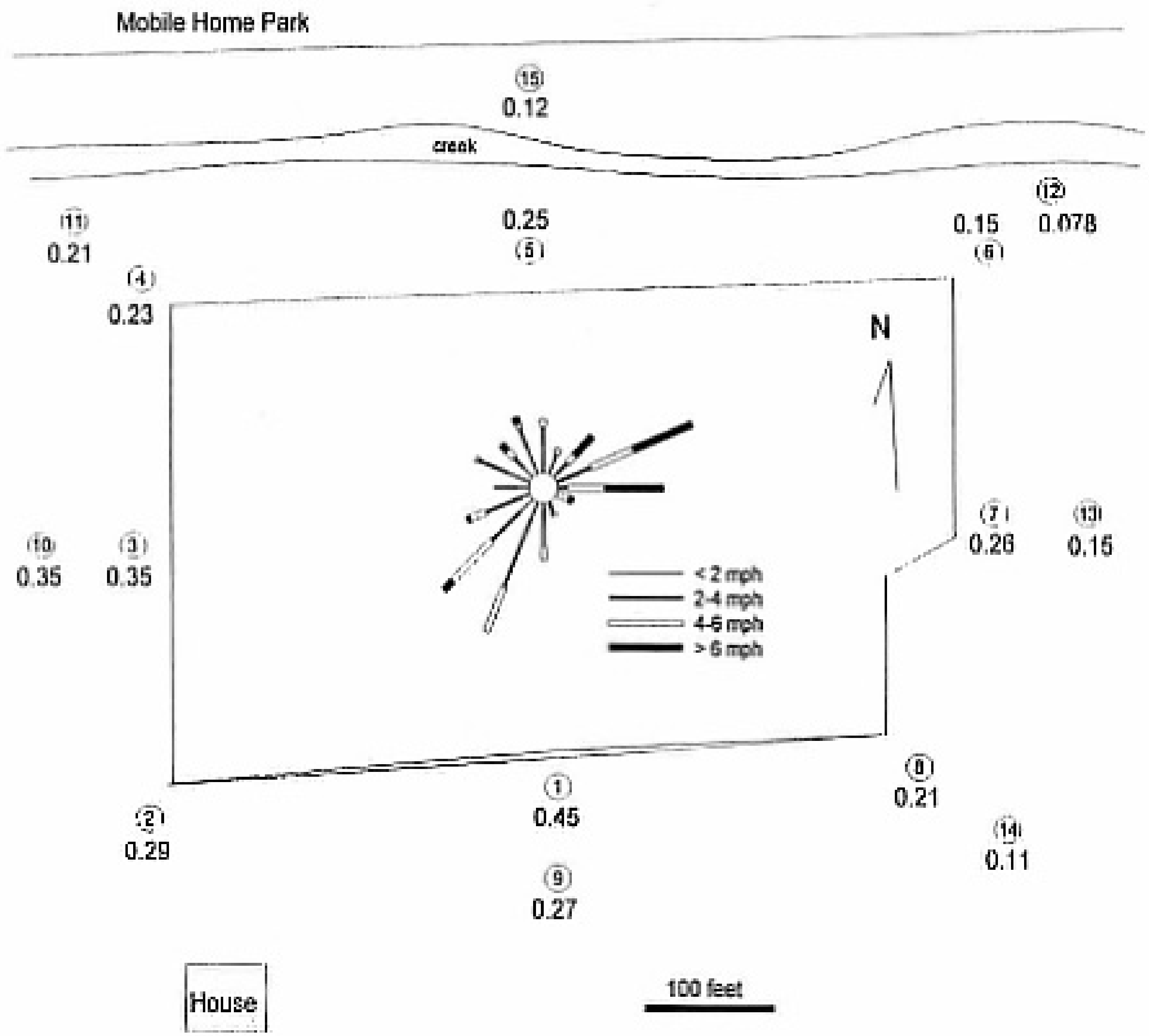


Table 1. Ambient methyl bromide air concentrations.

		Methyl Bromide (ppm) for each sampling period					
		Interval 1	Interval 2	Interval 3	Interval 4	Intervals l&2	Intervals 2&3
Site	Distance	11 Hour	12 Hour	12 Hour	12 Hour	23 Hour[1]	24 Hour[1]
1	28ft	**0.40**	**0.50**	0.072	0.12	**0.45**	**0.29**
2	32ft	0.17	0.39	0.011	0.11	0.29	0.20
3	3oft	0.20 (89%)	0.48	0.041 (72%)	**0.23**	0.35	0.26
4	30ft	0.14	0.30	0.056	0.14	0.23	0.18
5	33ft	0.27	0.23	**0.082**	0.088	0.25	0.16
6	34ft	0.25	0.062	0.029 (63%)	0.014	0.15	0.046
7	31ft	0.32	0.20	0.058	ND (65%)	0.26	0.13
8	36ft	0.21	0.21	0.049	0.023	0.21	0.13
9	98ft	0.23	0.31	0.025	0.074	0.27	0.17
10	101ft	0.27	0.42	0.021	0.23	0.35	0.22
11	100ft	0.13	0.29	0.029	0.16	0.21	0.16
12	101ft	0.093	0.063	0.011	0.014	0.078	0.037
13	103ft	0.20	0.10	ND	0.016	0.15	0.052[2]
14	119ft	0.096	0.12	0.025	0.018	0.11	0.074
15	165ft	0.083	0.16	0.018	0.036	0.12	0.088

(%) Percentage of interval sampled is given for truncated sample periods, due to pump/battery failure during sampling interval.

1 A two interval time weighted average concentration.

2 Indicates that the 24-hour average includes a period of no detectable amount, 0.0025ppm was used to obtain the 24-hour average.

ND = No detectable amount; reporting limit = 0.005 ppm

Bolded values are the highest concentrations for each column.

Mini-memo
To: Randy Segawa
From: Bruce Johnson
Subject: Preliminary Modeling Ocean0 site
cc: Kean Goh Date: November 16, 1998

These are the preliminary modeling results for the Oceano methyl bromide study (164-11) (Kim and Segawa 1998). If desired, I will provide a more complete memorandum.

I used ISCST3 to model 4 periods.

Period	Length (h)	Regression	Sorted Regression	Flux (ug/m2s)	
1	11	Ns	Did not sort**	NA	
2	12	P<.002, y=0.15 + .57x		57	Used for 24 hour avg. flux
3	12	Ns	P<.001, y= 0.0 + 0.60	60	Used for 24 hour avg. flux
4	12	P<.001, y=.05 + 0.19x		19	

**Application took place during over half of this period. Consequently, I did not think it appropriate to sort and regress.

I used periods 2 and 3 to calculate a 24 hour average flux rate of 58.5ug/m2s, I calculated 5 g/m2 was outgassed during this 24 hour period, which is 5/23=22% outgassing fraction. The 206 lbs./acre a-i. was equivalent to 23 g/m2 a.i. and was used in the denominator.

I simulated the 24 hour period, first as a coarse grid to determine where the maximum required buffer zone would be, then as a fine grid on the indicated field edge. The maximum required buffer zone was on the west side of the field and was 86 feet. This is consistent with Kim and Segawa (1998), who reported a 24 hour measured average concentration of 0.22 ppm at sampler 10 on the west side of the field, 101 feet away.

Reference

Kim, David and Randy Segawa. 1998. Memorandum to Douglas Y. Okumura on Monitoring results from a bedded, tarped, high barrier film, shallow injection methyl bromide application in San Luis Obispo County dated November 3, 1998.

D:\edrive\MEBR\oceano\oceanol.mem

D:\edrive\MEBR\oceano\periodl.mem January 19, 1999 (3:48PM)

Memorandum

To: Randy Segawa
From: Bruce Johnson
Subject: Estimating flux index for period 1, oceano study and associated 24 hour required buffer zone.
Date: January 15, 1999

You requested that I estimate the flux for period 1 in the Oceano study (Kim and Segawa 1998), even though in my original analysis of the Oceano data (Johnson 1998) I felt that there were compelling reasons not to use our normal approach to flux estimation for period 1. I have undertaken the following calculations to obtain a flux.

Unsorted regression.

	Msrd mm	Mdled Ug/m3	Msrd Ppb	Mdled Ppb
ROW	*c1*	*c2*	*c3*	*c4*
1	0.400	54.0	400	13.918
2	0.170	0.0	170	0.000
3	0.200	262.0	200	67.526
4	0.140	478.0	140	123.196
5	0.270	662.0	270	170.619
6	0.250	385.0	250	99.227
7	0.320	616.0	320	158.763
8	0.210	88.0	210	22.680
9	0.230	2.5	230	0.644
10	0.270	176.0	270	45.361
11	0.130	286.0	130	73.711
12	0.093	89.0	93	22.938
13	0.200	386.0	200	99.485
14	0.096	29.0	96	7.474
15	0.083	198.0	83	51.031

MTB > regr c3 1 c4   The regression equation is C3 = 180 + 0.372 C4

Predictor	Coef	Stdev	t-ratio	p
Constant	180.38	36.09	5.000	.000
c4	0.3724	0.4310	0.86	0.403

s = 90.58   R-sq = 5.4%   R-sq(adj) = 0.0%

Analysis of Variance

SOURCE	*DF*	*SS*	*MS*	*F*	*p*
Regression	*1*	*6128*	*6128*	*0.75*	*0.403*
Error	*13*	*106670*	*8205*		
Total	*14*	*112798*			

Unusual Observations

Obs.	*c4*	*c3*	*Fit*	*Stdev.Fit*	*Residual*	*St.Resid*
1	*14*	*400.0*	*185.6*	*31.8*	*214.4*	*2.53R*

R *denotes an obs. with a large st. resid.*

In this unsorted regression, the slope is not different from 0, while the constant is significantly different from 0. Next, I sorted c3 and c4, and redid the regression.

```
MTB > sort c3 cl3
MTB > sort c4 cl4
MTB > print cl3 cl4

ROW      Cl3         Cl4

1         83       0.000
2         93       0.644
3         96       7.474
4        130      13.918
5        140      22.680
6        170      22.938
7        200      45.361
8        200      51.031
9        210      67.526
10       230      73.711
11       250      99.227
12       270      99.485
13       270     123.196
14       320     158.763
15       400     170.619

MTB > regr cl3 1 cl4  The regression equation is Cl3 = 105 + 1.56 Cl4

Predictor        Coef        Stdev     t-ratio        p
Constant      104.842        8.340       12.57    0.000
Cl4           1.55698      0.09959       15.63    0.000

s = 20.93        R-sq = 94.9%       R-sq(adj) = 94.6%

Analysis of Variance

SOURCE          DF          ss        MS          F        p
Regression       1      107101    107101     244.40    0.000
Error           13        5697       438
Total           14      112798
```

This results in both the slope and intercept being significant. The statistical significance of a sorted regression cannot be interpreted the same way as in unsorted regression because preliminary simulation work indicates that almost all randomly chosen data will give significant regressions after sorting. However, in this case, the intercept is sizeable at 105 ppb, since the guideline for 24 hours is 210 ppb. A desperation measure, which we have considered using in situations where regressions are not working, is to simply sum up the measured values and sum up the modeled values and divide one number by the other.

In this case, this results in a ratio of 3.2, equivalent to a flux index of 320 ug/m2s. The calculations are outlined below this paragraph.

```
MTB > sum c3 kl
   SUM =          3062.0
MTB > sum c4 k2
   SUM =          956.57
MTB > let k3=kl/k2
MTB > prin k3
K3        3.20101
```

As a compromise, I tried regression, but forcing the line through the origin. This results in the following analysis.

```
MTB > regr cl3 1 c14;
SUB> noconstant.
```

The regression equation is
Cl3 = 2.51 Cl4

Predictor	Coef	Stdev	t-ratio	P
Noconstant				
Cl4	2.5105	0.2256	11.13	0.000

s = 73.17
Analysis of Variance

SOURCE	DF	ss	MS	F	p
Regression	1	662902	662902	123.82	0.000
Error	14	74952	5354		
Total	15	737854			

Unusual Observations

Obs.	Cl4	Cl3	Fit	Stdev.Fit	Residual	St.Resid
14	159	320.0	398.6	35.8	-78.6	-1.23 X
15	171	400.0	428.3	38.5	-28.3	-0.46 X

X denotes an obs. whose X value gives it large influence.

Since attempting to estimate flux during this period is dicey, due to the lack of relationship between the met data and the air concentrations, I believe the latter analysis represents the best compromise. This would result in a flux index of 251 ug/m2s for period 1.

Combining this flux index from period 1, with the previously calculated (Johnson 1998) flux index for period 2 gives a weighted average flux index of 150ug/m2s for the 23 hour combined length of periods 1 and 2.

$$\text{weighted avg} = \frac{11h \times 251\ \mu g/m^2s + 12h \times 57\ \mu g/m^2s}{23h} = 150\ \mu/m^2s$$

x

Using this average flux for the 23 combined 23 hour time period with ISCST3 (control file Table 1 and meteorological file Table 2) gives an indication that the largest buffer zone will be west of the field (Figure 1). A finer grid zeros in more closely to the required buffer zone (Figure 2) and gives an estimated required buffer zone of 94 meters or 308 feet.

References

Johnson, Bruce. 1998. Mini-memo to Randy Segawa on preliminary modeling Oceano site dated November 16, 1998.

Kim, David and Randy Segawa. 1998. Memorandum to Doug Okumura on Monitoring results from a bedded tarped, high barrier film, shallow injection methyl bromide application in San Luis Obispo County dated November 3, 1998.

D:\edrive\MEBR\oceano\periodl.mem January 19, 1999 (3:48PM)

Table 1.Control file for 23 hour combined periods 1 and 2 using 150ug/m2s flux index for Oceano study.

```
CO STARTING
CO TITLEONE Oceano periods l&2 23 hour simulation max buff
CO MODELOPT CONC RURAL          NOSTD NOBID NOCALM
CO AVERTIME PERIOD
CO POLLUTID OTHER
CO DCAYCOEF  .0000
CO FLAGPOLE 1.2
CO RUNORNOT RUN
CO ERRORFIL OCERR.OUT
CO FINISHED
SO STARTING
SO LOCATION   1 AREA            0.000     3.100   0.000
SO SRCPARAM   1 .000150    0.0 70.  109.2   0.  0.
SO LOCATION   2 AREA           70.        7.9      0.
SO SRCPARAM   2 .000150    0.0 40. 106.1  0.     0.
SO LOCATION   3 AREA           110.       9.9      0.
SO SRCPARAM   4 .000150    0.0 57.3  105.7  0.  0.
SO LOCATION   5 AREA           167.3     55.5      0.
SO SRCPARAM   6 4 .000150    0.0 16.2  61.3  0.    0.
SO EMISUNIT   .lOOOOE+7 (GRAMS/SEC)   (MICROGRAMS/CUBIC-METER)
SO SRCGROUP ALL
SO FINISHED
RE STARTING
RE GRIDCART MAXBUF STA
            XYINC       -200 19 25-200 19 25
RE GRIDCART MAXBUF END
RE FINISHED
ME STARTING
ME INPUTFIL OC24H.Pl2       (4IZ,2F9.4,F6.1,I2,2F7.1)
ME ANEMHGHT  10.000 METERS
ME SURFDATA  99999 1998       SURFNAME
ME UAIRDATA  99999 1998       UAIRNAME
ME WINDCATS   1.54 3.09 5.14 8.23 10.8
ME FINISHED
OU STARTING
OU PLOTFILE PERIOD ALL OC24Hlx.plt
OU FINISHED
```

Table 2. Meteorology file, OC24H.Pl2, for combined periods 1 and 2 simulations.

```
  99999      98   99999      98
9810 6 8 294.9111   1.1664 287.6 5     300.0    300.0
9810 6 9 351.8609   1.2163 292.6 4     300.0    300.0
9810 610 344.2586   2.1936 296.7 3     300.0    300.0
9810 611  72.7523   2.7084 298.6 2     300.0    300.0
9810 612  92.7406   2.8728 298.1 2     300.0    300.0
9810 613  89.4185   3.3880 298.1 3     300.0    300.0
9810 614  74.4658   2.9344 297.3 2     300.0    300.0
9810 615  80.5330   2.7372 296.9 2     300.0    300.0
9810 616  93.6403   1.9486 296.2 2     300.0    300.0
9810 617  79.3186   1.7215 297.3 2     300.0    300.0
9810 618  62.0765   1.1630 293.7 3     300.0    300.0
9810 619 261.2809   0.8206 289.9 4     300.0    300.0
9810 620 217.5560   1.4783 289.8 5     300.0    300.0
9810 621 213.7779   0.9587 287.7 6     300.0    300.0
9810 622 246.8420   1.9100 285.8 6     300.0    300.0
9810 623 229.5460   1.5516 286.9 6     300.0    300.0
9810 624 208.4444   1.7488 286.4 6     300.0    300.0
9810 7 1 282.4759   0.9637 283.9 6     300.0    300.0
9810 7 2 307.1960   0.7806 282.1 6     300.0    300.0
9810 7 3 246.9253   1.0652 283.3 6     300.0    300.0
9810 7 4 238.8274   1.4737 284.9 6     300.0    300.0
9810 7 5 262.6243   1.4596 282.9 6     300.0    300.0
9810 7 6 224.5218   2.1684 284.4 6     300.0    300.0
```

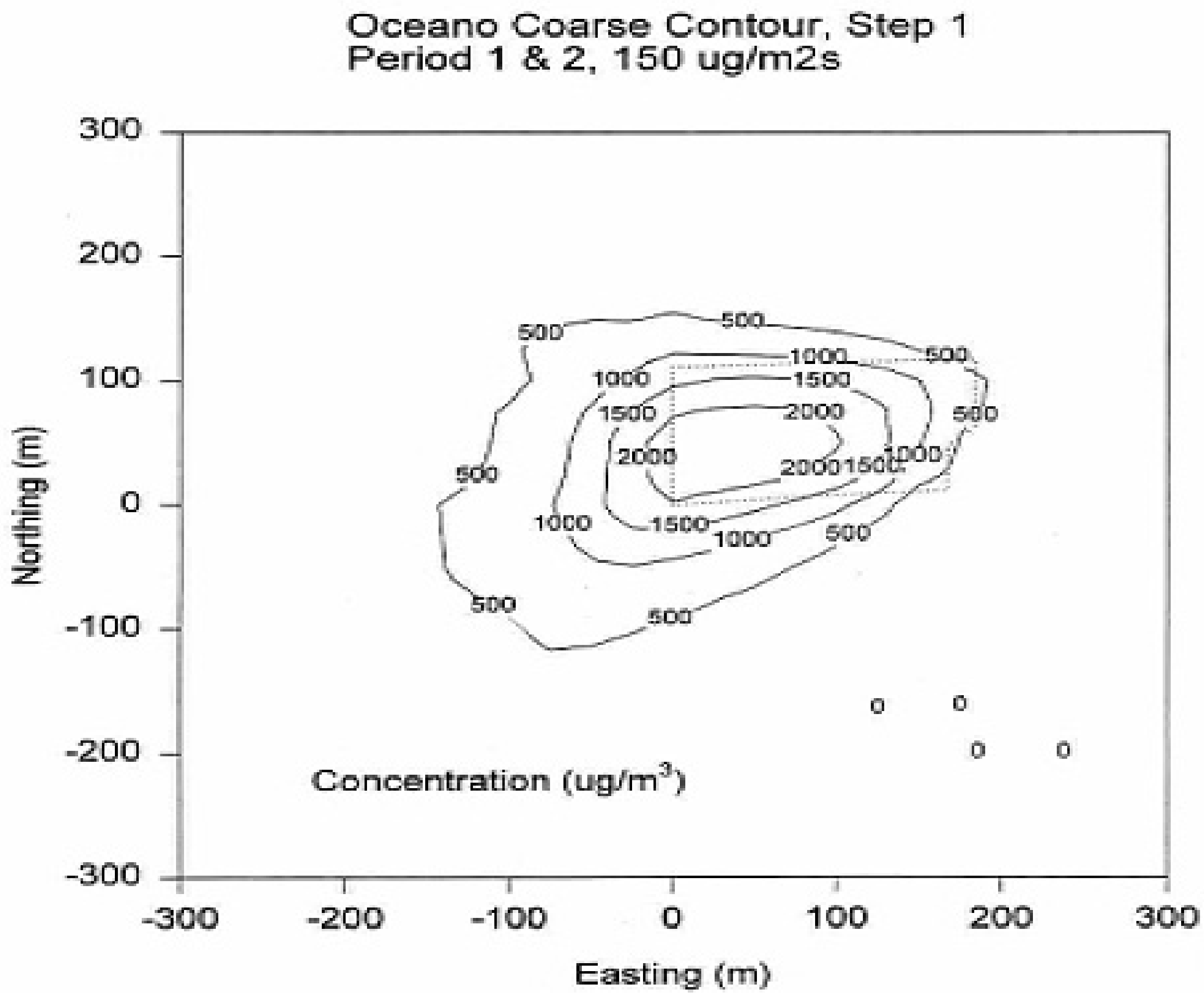


Figure 1. Coarse contour to locate direction of maximum buffer zone. Maximum direction west of field. Field indicated by dotted line in center.

d:\edrive\mebr\oceano\ocd24h1x.spw

Oceano Fine Contour, Step 2
Period 1& 2, 150 ug/m^{2}s

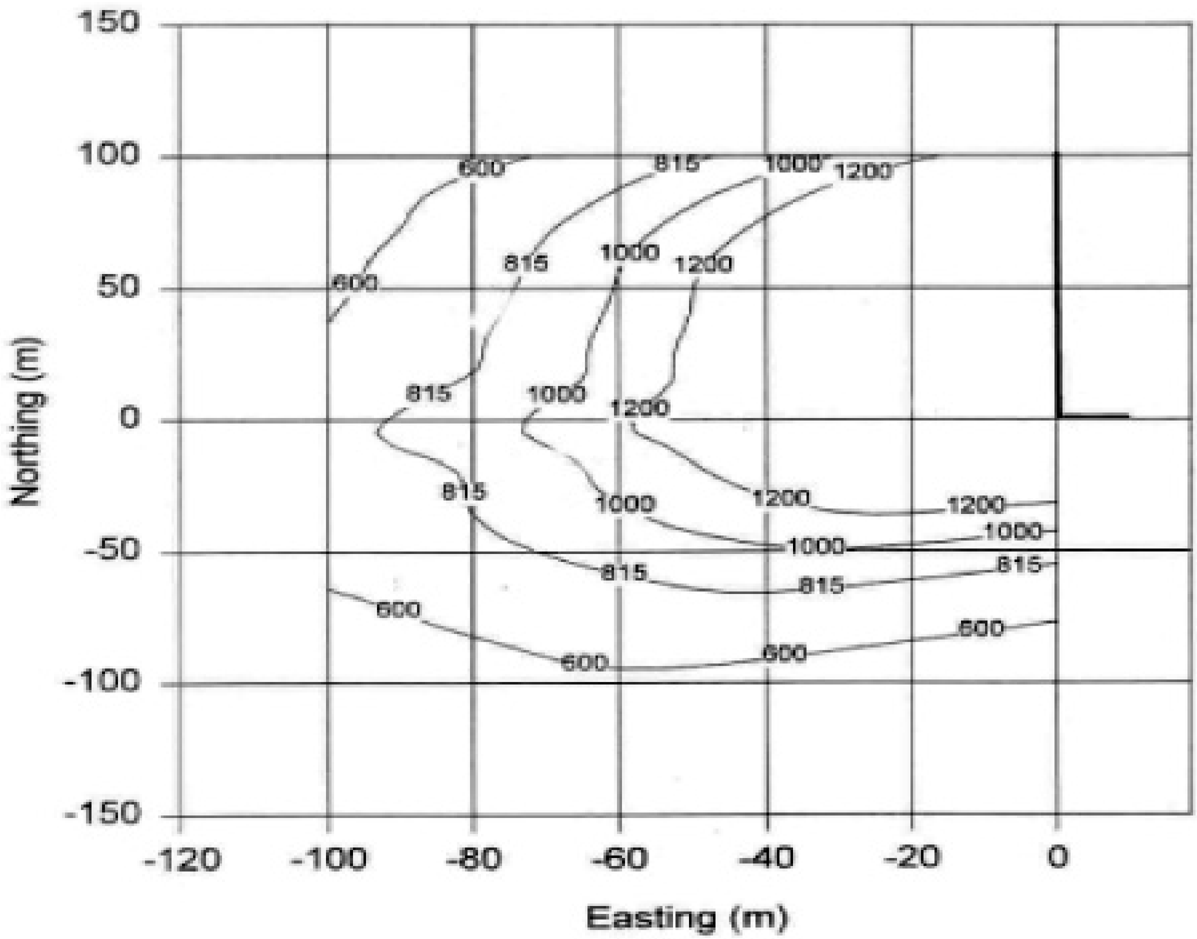


Figure 2. Finer grid to determine required buffer zone. Dark line indicates portion of west and southwest corner of field. Longest required bufferzone from SW corner to (-94,-5), giving length of 94m or 308 feet.

d:\edrive\mebr\oceano\oc24h2xb.spw

Mini-memo
To: Randy Segawa
From: Bruce Johnson
Date: February 8, 1999
Subject: Oceano mebr study

In the course of preparing the workbook on using the back calculation procedure and determining buffer zones, I discovered that the period 2 regression for the Oceano study had a significant intercept, a fact that I had previously overlooked. In thinking this through, however, I decided to compare the modeled versus measured values in the direction that the maximum buffer zone was determined in order to determine whether further analysis would be required in establishing this flux index and buffer zone. In this case, the direction was almost due west from the field (Johnson 1998, 1999). There were two monitors in this direction labeled as #3 and #10 (Kim and Segawa 1998, Figure 1.) I took the previously estimated (Johnson 1999) 24 hour flux index based on period 1 and 2 of 150ug/m2s and ran the model using the discrete receptors in order to compare the measured values for #3 and #10 against the modeled values with the estimated flux index for this 23 hour time period (d:\edrive\mebr\oceano\oc24hchk.out). The results were

Monitor	Coordinates	23 hr modeled conc		23 hr TWA msrd
Number	meters	ug/m3	ppm	ppm
#3	9.1,55.17	2139	0.55	0.35
#10	-30.8,55.2	1633	0.42	0.35

In other words, since using the estimated flux index results in the model overestimating the concentrations at these two receptors, which are in the direction of maximal concentrations from the field, the previously calculated required buffer zone of 308 feet (Johnson 1999) will be adequate. It is not necessary to further analyze this study.

Johnson, Bruce. 1999. Memorandum To: Randy Segawa From: Bruce Johnson Subject: Estimating flux index for period 1, oceano study and associated 24 hour required buffer zone. Date: January 15, 1999

Johnson, Bruce. 1999. Mini-memo To: Randy Segawa From: Bruce Johnson Subject: Preliminary Modeling Oceano Site cc Kean Goh Date November 16, 1998.

Kim, David and Randy Segawa. 1998. Memorandum to Doug Okumura on Monitoring results from a bedded tarped, high barrier film, shallow injection methyl bromide application in San Luis Obispo County dated November 3, 1998.

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Author: B. Johnson, T. Barry, and Pam Wofford

Document Date: September 1999

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APPROVED: ______________________ Date: 11/16/99
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Branch Chief